

ANDHRA UNIVERSITY
Department of Engineering Chemistry, AU College of Engineering (A)
5 YEAR INTEGRATED M.Sc. CHEMISTRY
(Specialization: APPLIED CHEMISTRY)
 (With Effect from the Admitted Batch of 2016-2017 Academic Year)
SCHEME OF INSTRUCTION AND EXAMINATION
SEMESTER IX (15 Weeks Duration)

Code Number	Course	Teaching/ Lab hours per week	Allotment of Marks		Total Marks	Credits
			External	Internal		
9T1/ Paper – I	Instrumental Methods of Analysis	4	70	30	100	4
9T2/ Paper – II	Organic Spectroscopy	4	70	30	100	4
9T3/ Paper – III	Organic Synthesis	4	70	30	100	4
9T4/ Paper – IV	Polymers and Plastics	4	70	30	100	4
9T5/ Paper – V	Medicinal Chemistry	4	70	30	100	4
9P1/ Practical- I	Organic Chemistry Practical	6	100	50	150	4
9P2/ Practical- II	Quantitative Analysis Practical	6	100	50	150	4
9S1	Seminar Presentation			50	50	2
				Total	850	30

Total Credits for IX Semester

Theory	: 20
Practical & Seminar	: 10
Total	: 30

SYLLABUS
IX SEMESTER
9T1/ PAPER-I: INSTRUMENTAL METHODS OF ANALYSIS

UV-Visible Spectrophotometry: Principle, Beer -Lambert's Law, Instrumentation, Advantages, Applications and Limitations - Single and Double beam spectrophotometers, Analysis of mixtures

Atomic Absorption Spectrometry (AAS), Flame Photometry (AES), Fluorimetry, Nephelometry and Turbimetry - Basic Principles, Theory, Instrumentation and Applications

Chromatography Methods: Principles of Separation and Classification

Paper Chromatography: Definition, Principles and Applications of paper chromatography;

Thin Layer Chromatography: Definition, mechanism, efficiency of TLC plates, Selection of stationary and mobile phases;

Gas Chromatography – Instrumentation: Carrier gas, columns, stationary phases and detectors used in GC, Some qualitative and quantitative applications of GC: Analysis of chlorinated pesticides in water and trihalomethanes in drinking water;

High Performance Liquid Chromatography – Instrumentation: Columns, stationary phases, Mobile phases and detectors used in HPLC, Some qualitative and quantitative applications of HPLC: Determination of Aspirin, Phenacetin and Caffeine in mixture; Determination of Fluoxetine in Serum; GC-MS and LC-MS: Techniques and applications

Ion-Exchange Methods: General discussion, Typical synthetic Cation and Anion exchange resins. Action of ion exchange resins. Ion-exchange equilibria, Ion-exchange capacity, Determination of cation and anion exchange capacity, Column operation and ion exchange chromatography, Separation of Zn and Mg using anion exchange resin, Determination of total cation concentration in water.

Thermal Methods of Analysis: Principles, Instrumentation, Comparison and interpretation of TGA and DTG curves, TGA curves of mixtures, Factors affecting TGA curves, Applications of TGA. Differential Thermal Analysis and Differential Scanning Calorimetry - Principles, Instrumentation and quantitative aspects of DTA and DSC curves; Interpretation of DTA and DSC curves. Influence of atmosphere on DTA curves of a sample, Complementary nature of TGA and DTA Applications of DTA and DSC

Suggested books:

1. Vogel's Text book of quantitative chemical analysis; G. H. Jeffery et. al. Addison Wesley Longman
2. Instrumental methods of analysis, H.H. Willard, L.L. Merritt, Jr., J.A. Dean and F.A. Settle, Jr., Van Nostrand Reinhold Co., New York
3. Modern analytical chemistry; David Harvey; McGraw Hill
4. Principles and practice of analytical chemistry; F. W. Fifield & D. Kealey, Blackwell Science
5. Automatic methods of analysis, M. Valcarcel, M. D. Luque de Castro, Elsevier, Vol. 9
6. Principles of Instrumental Analysis, Skoog, Holler and Wieman, Harcourt Asia

9T2/ PAPER-II: ORGANIC SPECTROSCOPY

Infrared Spectroscopy : Units of frequency, wave length and wave number-molecular vibrations-factors influencing vibrational frequencies of organic molecules and interpretation of spectra .

Ultraviolet Spectroscopy : Introduction ,the absorption laws ,measurement of the spectrum, chromophores, standard works of reference, definitions, applications of UV spectroscopy to conjugated dienes, trienes, unsaturated carbonyl compounds and aromatic compounds .

Nuclear Magnetic Resonance Spectroscopy:

Proton (^1H) – NMR: Introduction , basic principles, the chemical shift, the intensity of NMR signals - factors affecting the chemical shifts- spin-spin coupling. some simple splitting patterns- the magnitude of coupling constants-first order spectrum-interpretation of spectra . Chemical shift reagents- nuclear Overhauser effect (NOE).The Fourier transform technique.

Carbon -13 NMR : Introduction -Spin decoupling- chemical shifts - interpretation of spectra . The DEPT experiment.

Mass Spectroscopy : Basic principles : instrumentation : the mass spectrometer , isotope abundances, the molecular ion ,meta stable ions. Fragmentation processes-mass spectra of some chemical classes-interpretation of spectra .

Suggested books:

1. Spectroscopic methods in Organic chemistry . Forth Edition D.M williams and I. Flemings Tata –McGraw Hill , New Delhi
2. Organic Spectroscopy ,W.Kemp ,ELBS Macmillan

Reference Books

1. Applications of Absorption Spectroscopy of Organic Compounds J. R. Dyer , Prentice Hall of India, New Delhi ,1984 .
2. Spectrometric Identification of Organic Compounds , Sixth Edition, R.M Silverstein ; F.X.Webster, John Willey ,Singapore.

9T3/ PAPER-III: ORGANIC SYNTHESIS

Formation of Carbon – Carbon Single Bonds : alkylation via enolate, the enamine and related reactions, umploung (dipole inversion) – the aldol reaction –applications of organo palladium , organo nickel and organo copper reagents- applications of α -thiocarbanions, α -selenocarbanions and sulphur ylids -synthetic applications of carbenes and carbenoids.

Formation of Carbon – Carbon Double Bonds: β -Elimination reactions, pyrolytic syn eliminations, sulphoxide –sulphenate rearrangement- the wittig and related reactions- alkenes from arylsulphonylhydrazones –claisen rearrangement of allyl vinyl ethers.

Reactions of unactivated carbon-hydrogen bonds: The Hoffmann-Loeffler –Freytag reaction – The Barton reaction –Photolysis of organic hypohalites .

Synthetic applications of Organo boranes: Organo boranes : Preparation of organo boranes viz hydroboration with BH_3 –THF ,dicylohexyl borane , disiamyl borane ,thexyl borane, 9-BBN and di-isopinocampheyl borane. Functional group transformations of organo boranes: oxidation, protonolysis and rearrangements .Formation of carbon - carbon bonds viz organo boranes carbonylation ,the cyanoborate process and reaction of alkenyl boranes.

Synthetic Applications of Organo silanes: Organo silanes : Synthetic applications of trimethylsilyl chloride, dimethyl –t-butylsilyl chloride , trimethylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate. Synthetic applications of α -silyl carbanions and β -silyl carbonium ions.

Phase Transfer Catalysis: Phase transfer catalysis –principle and applications.

Oxidation : Oxidations of hydrocarbons , alkenes , alcohols aldehydes and ketones oxidative coupling reactions . Use of $Pb(OAc)_4$, NBS, CrO_3 , SeO_2 , MnO_2 , alkoxyulphonium salts, $KMnO_4$, OsO_4 , RuO_4 , peracid and $Tl(III)$ nitrate .

Reduction: Catalytic hydrogenation(homogeneous and heterogeneous),reduction by dissolving metals , reduction by hydride transfer reagents, reduction with hydrazine and diimide ,selectivity in reduction of nitroso and nitro compounds , reductive cleavage .

Design of Organic synthesis : Retrosynthesis - The Disconnection Approach – Basic Principles Convergent and Linear Synthesis .

Suggested books:

1. Modern Methods of Organic Synthesis by W.Carruthers
2. Modern Synthetic Reactions by H. O. House
3. Organic Synthesis by Robert & Ireland
4. Designing Organic Synthesis by B Staurt Warron
5. Organic Synthesis by S.Warrant

9T4/ PAPER-IV: POLYMERS AND PLASTICS

Polymers: Basic concepts Nomenclature- Degree of polymerization – polymerisation process – Classification of polymerization reactions – Difference between thermoplastics and thermosets. Types of polymerization – Addition and step growth. Copolymerisation- Block copolymerisation – Graft copolymerisation. Stereo isomers – isotactic, atactic and syndiotactic polymers. Mechanism of polymerization – free radical and ionic. Heterogeneous polymerization – Zeigler-Natta catalysis. Compounding of plastics – Fabrication techniques of plastic.

Polymer Degradation: Polymer degradation – Types of degradation – thermal, mechanical, ultrasonic waves, photo-degradation, oxidative degradation (rubber and phenol-formaldehyde) and hydrolytic degradation.

Kinetics of Polymerisation Reaction: Addition – Free-radical, Cationic and Anionic polymerization. Condensation polymerization – acid catalysed condensation reactions.

Analysis and Testing of Polymers: Weight average and Number average molecular weights of polymers - Ratio of M_w and M_n . Determination of molecular weight of polymers by Cryoscopy – Light scattering – X-ray scattering – Viscosity – Ultra centrifuge and gel permeation chromatographic methods.

Rubbers, Elastomers and Adhesives: Origin and Chemical structure of natural rubber – Direct Processing of Latex – Compounding of rubber – Fabrication of rubber – Vulcanization of rubber. Elastomers – Manufacture, properties and uses of Butadiene, Isoprene and chloroprene. Natural and synthetic adhesives - Classification animal glue. Protein and starch adhesives – Resin adhesives. Difference between plastics, elastomers and adhesives.

Suggested Books:

1. Petroleum products Hand Book, Virgil.B Guthrie, Editor, 1st ed Mc Graw Hill book company Inc 1960
2. Chemicals from petroleum , A. L. Waddns and J. Murray, ELBS Edn. 1970
3. Introduction to polymer chemistry, Raymond B, Seymour.
4. Polymer science, V.R. Gowariker et al ., New Age Intl (P)Ltd, New Delhi.
5. Organic chemistry of synthetic High Polymers, Robert W. Lenz, Interscience Publishers.
6. Chemical process Industries 5th Ed , George T. Austin, Mc Graw- Hill company Inc 1984.
7. Industrial chemistry by B k sherma 5th Ed 1993.
8. Textbook of Polymer Science P. W. Billmeyer, John Wiley, 1962

9T5/ PAPER-V: MEDICINAL CHEMISTRY

Drug Design: Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of pro-drugs and soft- drugs, structure activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50.

Pharmacokinetics: Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

Pharmacodynamics: Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

Antineoplastic Agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Cardiovascular Drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol,

Local Antiinfective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapson, amino salicylic acid and chloroquin.

Psychoactive Drugs: Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, phenytoin, ethosuximide, barbiturates, thiopental sodium, glutethimide.

Antibiotics: Cell wall biosynthesis, inhibitors, β -lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxicillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin.

Suggested Books:

1. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F.Dorge.
3. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter.-9 and Ch-14), Ed. M. E. Wolff, John Wiley.
4. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
5. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.

9P1/ PRACTICAL-I: ORGANIC CHEMISTRY PRACTICAL

Organic Mixture Analysis

1. Separation of organic compounds of a mixture (minimum of four mixtures)
2. Systematic identification of the separated organic compounds by functional group analysis, chemical reaction and derivatisation
3. Separation of organic compounds of a mixture by TLC

Reference Books:

1. A Text book of practical organic chemistry, A.I. Vogel, ELBS.
2. Laboratory Manual of Organic Chemistry by Raj K Bansal

9P2/ PRACTICAL-II: QUANTITATIVE ANALYSIS PRACTICAL

POTENTIOMETRY

1. Determination of Iron (II) with chromium (VI) .
2. Determination of Iron (II) with cerium (IV) .
3. Determination Vanadium (V) with Iron (II) .

pH METRY

4. Titration of a strong acid against a strong base.
5. Titration of a weak acid against a strong base .
6. Titration of a mixture of weak acid and a strong acid against a strong base.

CONDUCTOMETRY

7. Titration of a weak acid against a strong base.
8. Determination of percentage purity of AgNO_3 Solution using KCl .

COLOURIMETRY

9. Determination of Manganse .
10. Determination of Fe (II) .

Reference Books:

1. A text book of Practical Inorganic Chemistry by AI Vogel, ELBS
2. Laboratory manual of Engineering Chemistry by Dr Sudha rani

MODEL QUESTION PAPER

5 YEAR INTEGRATED M.Sc. CHEMISTRY

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IX SEMESTER

Paper I: INSTRUMENTAL METHODS OF ANALYSIS

Time: 3 Hours

Max. Marks: 70

*Answer any FIVE questions.
All questions carry equal marks*

- 1 Explain the principle, instrumentation and application of UV-Visible spectroscopy
- 2 Write notes on the following
 - (a) Flame Photometry
 - (b) Atomic Absorption Spectrometry
- 3
 - (a) Give the principle and application of Thin Layer Chromatography
 - (b) Explain instrumentation in Gas Chromatography
- 4
 - (a) Explain the Principle and Instrumentation of HPLC
 - (b) Briefly explain the application of GC-MS
- 5
 - (a) Explain the methods involved in determination of Aspirin, Phenacetin and Caffeine in mixture using HPLC
 - (b) Explain the method of determination of total cation concentration in water
- 6
 - (a) What are ion exchange resins? Explain the method of determination of ion-exchange equilibrium
 - (b) Briefly explain the determination of ion exchange capacity
- 7
 - (a) Explain the Instrumentation and Application of TGA
 - (b) Compare DTA and DSC curves

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Paper II: ORGANIC SPECTROSCOPY

Time: 3 Hours

Max. Marks: 70

*Answer any FIVE questions.
All questions carry equal marks*

- How do you distinguish the following by using IR spectra
 - Cis and Trans 2-butene
 - Ethanol and dimethyl ether
 - $C_6H_5COOCH_3$ and $CH_3COOC_6H_5$
 - $(CH_3)_3N$ and $CH_3-CH_2-CH_2-NH_2$
- Explain the functional group and finger print regions
 -
- Explain chromophores, auxochromes and Bathochromic and hypsochromic shifts with suitable examples
- Explain Nuclear Overhauser Effect, Geminal and Vicinal Couplings and ROSSY
- How would you distinguish o- and m- anisidines on the basis mass spectral studies
 - Explain the fragmentation process of cyclohexanone and acetophenone
- Explain Base peak, Molecular ion and Fragmentation ions
 - Explain isotope abundance and metastable ions
- An organic compound gave the following spectral data. Deduce the structure of the compound
Mass (m/z): 73, 91, 149, 164
IR ν (cm^{-1}): 1730
 1H NMR δ ppm: 2.0 (3H, s); 2.93(2H, t J=7 Hz); 4.30 (2H, t J= 7 Hz); 7.30 (5H, s)

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IX SEMESTER

Paper III: ORGANIC SYNTHESIS

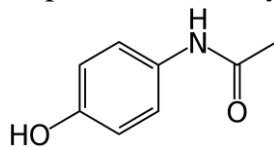
Time: 3 Hours

Max. Marks: 70

Answer any FIVE questions.

All questions carry equal marks

- Explain the alkylation via enolates and enamines with two examples each
 - Write the synthetic applications of α -thiocarbanions, organo nickel reagents and carbenes with one example each
- Explain the formation of C=C bonds by Wittig reaction and Claisen rearrangements. Give mechanisms
 - Explain HLF reaction and Barton Reaction with an example each
- Write the preparation and synthetic application of BH_3 -THF, 9-BBN and disiamyl borane
 - Write the preparation and synthetic applications of trimethylsilyl chloride and trimethylsilyl triflate
- Explain the oxidation of hydrocarbons, alkenes and aldehydes with suitable reagents and give their mechanisms
 - Write the preparation and applications of CrO_3 and Peracid
- Explain the reduction by dissolving metals and hydride transfer reagents and give their mechanisms
 - Explain the selectivity in reduction of nitroso and nitro compounds
- Explain the principle and application of Phase Transfer Catalysis with examples
 - Explain the Retrosynthesis for the following compounds



and

- Write short note for the following
 - Umpolung reaction
 - β -elimination reactions
 - Reaction of alkenyl borane

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IX SEMESTER

Paper IV: POLYMERS AND PLASTICS

Time: 3 Hours

Max. Marks: 70

*Answer any FIVE questions.
All questions carry equal marks*

- 1 (a) Explain the differences between thermoplastics and thermosets.
(b) Describe the various methods involved in co-polymerization.
- 2 Briefly explain the following.
(a) Atactic and syndiotactic polymers.
(b) Fabrication techniques of plastic.
(c) Zeigler-Natta catalysis.
- 3 Explain the mechanism involved in mechanical, thermal and oxidative degradations with examples.
- 4 (a) Describe the different types of degradation involved in hydrolytic degradation.
(b) Explain the influence of ultrasonic waves on polymer degradation and stability factors.
- 5 (a) Describe the kinetics of polymer reactions in addition and free radical reactions.
(b) Explain how the condensation reactions are catalysed by acids? Give examples.
- 6 How do you determine the molecular weight of polymers by ultra centrifuge, gel permeation chromatographic and X-Ray scattering methods?
- 7 (a) How do you determine the direct processing of latex.
(b) What are elastomers and adhesives? Explain their manufacture, properties and uses.

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IX SEMESTER

Paper V: MEDICINAL CHEMISTRY

Time: 3 Hours

Max. Marks: 70

*Answer any FIVE questions.
All questions carry equal marks*

- 1 (a) Explain different procedures adopted in drug design
(b) Outline the fundamental principles of SAR and QSAR
- 2 (a) Explain the concepts of prodrugs and soft drugs
(b) Explain the concepts of LD-50 and ED-50
- 3 (a) Explain the process of drug absorption and drug elimination
(b) Explain the application of pharmacokinetics in drug development process
- 4 (a) Write short notes on enzyme stimulation
(b) Explain the importance of drug metabolism in medicinal chemistry
- 5 (a) Explain the role of alkylating agents in the treatment of cancer
(b) Write the synthesis of Mechlorethamine and Uracil
- 6 (a) Explain the chemistry and mode of action of Quinidine and Diltiazem
(b) Write the synthesis of Sulphonamide and Aminosalicic acid
- 7 (a) What are antibiotics? Write a note on cell-wall biosynthesis
(b) Explain the chemistry and mode of action of CNS depressants and anti-anxiety drugs