ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

M.Sc. Chemistry

(For the students admitted during the academic year 2024–2025 onwards)

SEMESTER - I										
S. No	**Core /Elective**	**Code**	**Title of the Course**	**L**	**T**	**P**	**Credits**	**IA**	**SEE**	**Total Marks**
1	Core-theory	24MCHE11T	Inorganic chemistry – I	4	-	-	4	20	80	100
2	Core-theory	24MCHE12T	Organic chemistry – I	4	-	-	4	20	80	100
3	Core-theory	24MCHE13T	Physical chemistry – I	4	-	-	4	20	80	100
4	Elective	24MCHE1AT	General topics in chemistry	4	-	-	4	20	80	100
		24MCHE1BT	Pharmaceutical quality control and quality assurance							
5	Core practical	24MCHE11L	Inorganic chemistry practicals	-	-	8	4	20	80	100
6	Core practical	24MCHE12L	Organic chemistry practicals - I	-	-	8	4	20	80	100
			Total				26	120	480	600

SEMESTER - II										
S. No	**Core /Elective**	**Code**	**Title of the Course**	**L**	**T**	**P**	**Credits**	**IA**	**SEE**	**Total Marks**
1	Core-theory	24MCHE21T	Inorganic chemistry – II	4	-	-	4	20	80	100
2	Core-theory	24MCHE22T	Organic chemistry – II	4	-	-	4	20	80	100
3	Core-theory	24MCHE23T	Physical chemistry – II	4	-	-	4	20	80	100
4	Elective	24MCHE2AT	Applied and environmental aspects	4	-	-	4	20	80	100
		24MCHE2BT	Chemistry in day-to-day life							
5	Core practical	24MCHE22L	Organic chemistry practicals - II	-	-	8	4	20	80	100
6	Core practical	24MCHE23L	Physical chemistry practicals	-	-	8	4	20	80	100
			Total				26	120	480	600

SEMESTER - III										
S. No	**Core /Elective**	**Code**	**Title of the Course**	**L**	**T**	**P**	**Credits**	**IA**	**SEE**	**Total Marks**
1	Core-theory	24MCHE31T	Inorganic chemistry – III	4	-	-	4	20	80	100
2	Core-theory	24MCHE32T	Organic chemistry – III	4	-	-	4	20	80	100
3	Core-theory	24MCHE33T	Physical chemistry – III	4	-	-	4	20	80	100
4	Elective	24MCHE3AT	Drug discovery, design and development.	4	-	-	4	20	80	100
		24MCHE3BT	Materials Science							
5	Core practical	24MCHE34L	Multistep synthesis of organic compounds	-	-	8	4	20	80	100
6	Core practical	24MCHE35L	Molecular drawing, modeling, synthesis and characterization of selected bioactive molecules	-	-	8	4	20	80	100
			Total				26	120	480	600

SEMESTER - IV										
S. No	**Core /Elective**	**Code**	**Title of the Course**	**L**	**T**	**P**	**Credits**	**IA**	**SEE**	**Total Marks**
1	Core-theory	24MCHE41T	Organic chemistry – IV	4	-	-	4	20	80	100
2	Core-theory	24MCHE42T	Organic Spectroscopy	4	-	-	4	20	80	100
3	Core-theory	24MCHE43T	Medicinal chemistry and natural products	4	-	-	4	20	80	100
4	Elective	24MCHE4AT	Industrial organic chemistry	4	-	-	4	20	80	100
		24MCHE4BT	Bioinorganic, bioorganic, biophysical chemistry							
5	Core practical	24MCHE44L	Spectral identification of organic compounds	-	-	8	4	20	80	100
6	Project work	24MCHE45P	Project work	-	-	8	4			100
			Total				26	120	480	600

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Title of the Course: Inorganic chemistry - I
Category: Core-theory
Course Code: 24MCHE11T
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide students with an in-depth understanding of metal-ligand bonding theories, as well as the equilibrium concepts and applications of HSAB theory. It covers key reaction mechanisms, including substitution, acid and base hydrolysis, and electron transfer reactions. Additionally, students will learn about the preparation, structure, and bonding of carbonyl and nitrosyl complexes, along with metal atom clusters.

Course Outcomes:
At the end of the course, the student will be able to
1. describe crystal field theory and its applications in transition metal complexes.
2. analyze factors affecting metal-ligand complex stability using HSAB theory.
3. evaluate kinetics and mechanisms of substitution reactions in metal complexes.
4. integrate knowledge of bonding and structures in metal carbonyls, nitrosyls, and atom clusters.

Unit 1 Metal-ligand bonding theories 15

Crystal field theory (CFT) for bonding in transition metal complexes; crystal field splitting of d-orbitals in octahedral, tetrahedral, tetragonal and square planar fields; crystal field stabilization energy (CFSE) and its calculation in six and four coordinated complexes; spectrochemical series with reference to ligands and metal ions; factors affecting the magnitude of Δ_O in octahedral complexes; Jahn–Teller effect and its consequences; shortcomings of CFT; covalency: evidence for covalency, Nephelauxetic effect; applications of crystal field theory – structure of spinels (normal and inverse); octahedral site specific energy (OSSE); molecular orbital theory: concept of ligand groups orbitals (LGOs), MO diagrams for octahedral, tetrahedral and square planar complexes, and MO treatment of π-bonds.

Unit 2 Metal-ligand equilibria in solution and theory of HSAB 15

Metal-ligand Equilibria in solution. Stepwise and overall formation constants and their interrelationship; trends in stepwise formation constants; factors affecting the stability of metal complexes; chelate effect; determination of binary formation constants by p^H-metry and spectrophotometric methods.
Theory of HSAB. Hard and soft acids and bases; classification; acid-base strength and hardness; symbiosis; electronegativity and hardness; application of HSAB: biological functions and toxicology of metals, and medicinal applications.

Unit 3 Reaction mechanisms of complexes 15

Reactivity of metal complexes; inert and labile complexes; kinetics and mechanisms of substitution reactions; kinetics of substitution reactions in octahedral complexes; acid hydrolysis and factors affecting acid hydrolysis; base hydrolysis; conjugate base mechanism; anation reactions; substitution reactions in square planar complexes; trans effect and mechanism of trans effect; electron transfer reactions, inner sphere and outer sphere mechanisms and Marcus theory.

Unit 4 Carbonyl and Nitrosyl complexes, and metal atom clusters 15

Metal Carbonyl and Nitrosyl Complexes. Metal carbonyls: preparation of metal carbonyls of Mn, Fe, Co and Ni, bonding in carbonlys, EAN and 18-electron rule in carbonyls, π-bonding in carbonyls, terminal and bridging carbonyls, measurement of π-bond strength in carbonyls, structures of mononuclear, binuclear, trinuclear and tetranuclear carbonyls; metal nitrosyls: chemistry of linear and bent nitrosyls, nitrosyls as NO^+ and NO^- donors, analytical uses of nitrosyl complexes.

Metal Atom Clusters. Cage structures, higher boranes, carboranes, metal-metal bonds in carbonyl cluster, LNCCs and HNCCs, isoelectronic and isolobal relationships, hetero atom in metal atom clusters, electron counting schemes for HNCCs, HNCCs of Fe, Co, Ni, Ru, Rh, Pd, Os, Ir and Pt, lower halide and chalcogenide clusters, triangular clusters, solid state extended arrays.

Prescribed Textbooks:

1. Cotton, F. A., Wilkinson, G., Bochmann, M. *Advanced Inorganic Chemistry*. 6th Ed., John Wiley & Sons, 1999.
2. Huheey, J. E., Keiter, E. A., & Keiter, R. L. *Inorganic Chemistry: Principles of Structure and Reactivity*. 4th Ed., Prentice Hall, 2014.

Reference Books:

1. Lee, J. D. *Concise Inorganic Chemistry*. 5th ed., Wiley-Blackwell, 2014.
2. Jolly, W. L. *Modern Inorganic Chemistry*. 2nd ed., McGraw-Hill, 1991.
3. Kettle, S. F. *Coordination Compounds*. Springer, 2010.
4. Wulfsberg, G. *Inorganic Chemistry*. University Science Books, 2000.
3. Figgis, B. N. *Introduction to Ligand Fields*. Krieger Pub Co., 1984.

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Title of the Course: Organic chemistry - I
Category: Core-theory
Course Code: 24MCHE12T
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide a comprehensive understanding of the fundamental concepts of aromaticity in organic molecules and the mechanisms involved in various organic reactions. It covers the preparation, geometry, and stability of reaction intermediates, along with in-depth knowledge of aliphatic and aromatic nucleophilic and electrophilic substitution reactions. Additionally, the course introduces students to the concepts of chirality in stereoisomers and offers insight into conformational analysis.

Course Outcomes:
At the end of the course, the student will be able to
1. explain localization, delocalization, and resonance in aromatic compounds using Hückel's rule.
2. analyze reaction mechanisms and predict the stability of reactive intermediates in organic reactions.
3. differentiate substitution reactions by evaluating mechanisms, energy profiles, and stereochemistry.
4. assess stereochemical properties and stability of molecules with chiral centers and conformational variations.

Unit 1 Aromaticity **15**

Localization, delocalization, conjugation, resonance, the energy, structural and electronic criteria for aromaticity; relationship among energetic, structural and electronic criteria; Huckle's rule and molecular orbital theory, aromaticity in benzenoid and non-benzenoid compounds; aromaticity in charged ring fused-ring systems; heteroaromatic systems; annulenes: cyclobutadiene, benzene,1,3,5,7- cyclooctatetraene, [10] annulenes-1,3,5,7,9-cyclodecapentaene isomers, and [12]-, [14]-, [16]- and [18]- annulenes; azulenes; fulvenes; fullerenes; ferrocene; anti-aromaticity; homo-aromaticity.

Unit 2 Reaction mechanism and reactive intermediates **15**

Reaction Mechanism. Types of bond cleavage; general classification of organic reactions; potential energy diagrams; thermodynamic requirements; kinetic requirements; kinetic and thermodynamic control; general methods of determination of reaction mechanism.
Reactive Intermediates. General methods of generation, geometry, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes

Unit 3 Substitution reactions **15**

General introduction, classification of substitution reactions.
Nucleophillic Substitutions. i. Aliphatic nucleophillic substitutions. S_N1 and S_N2 reactions: mechanism, energy profile diagram and stereochemistry; SET and S_Ni mechanisms; neighbouring group participation: criteria for determining the participation of neighbouring group, neighbouring group participation involving oxygen, sulphur, nitrogen, aryl, σ and π- bonds. ii. Aromatic nucleophilic substitution. Introduction; S_NAr and benzyne mechanisms; von Richter, Sommelet-Hauser and Smiles rearrangements.
Aromatic Electrophilic Substitutions. Introduction; arenium ion mechanism-S_E2 reaction; orientation and reactivity; energy profile diagram; diazonium coupling; Vilsmeier reaction; Gattermann-Koch reaction; Pechman reaction; Reimer-Tiemann reaction

Unit 4 Stereochemistry and conformational analysis 15

Concept of Chirality. Definitions: enantiomer, diastereomer, invertomer, homomer, epimer, anomer; R,S nomenclature; molecules with single chiral center: tricoordinate and tetracoordinate; molecules with two and more chiral centers: constitutionally unsymmetrical and symmetrical, erythro – threo nomenclature

Aspects of Geometrical Isomerism (π-Diastereoisomerism). Cis-trans, and E-, Z- nomenclature; methods of determining configuration of geometrical isomers using physical, spectral and chemical methods; stability; cis-trans interconversion.

Stereoisomerism in Molecules without Chiral Center. Axial chirality: Allenes, alkylidenecycloalkanes, spiranes, nomenclature. Atropisomerism: Biphenyl derivatives, nomenclature. Planar Chirality: Ansa compounds, paracyclophanes, trans-cyclooctene, helicity.

Conformational Analysis. 2,3-dimethylbutane; conformation and intramolecular hydrogen bonding: ethylene glycol, 2-chloroethanol; 2,3-dibromobutane; butane-2,3-diol; disubstituted cyclohaxanes; cyclohexene; cyclohexanone; decalin; 9-methyldecalin.

Prescribed Textbooks:

1. Smith, Michael B., and Jerry March. *Advanced Organic Chemistry: Reactions, Mechanism, and Structure*. 6th ed., John Wiley & Sons.
2. Carey, Francis A. *Organic Chemistry*. 4th ed., McGraw-Hill Higher Education.

Reference Books:

1. Miller, Bernard. *Advanced Organic Chemistry: Reactions and Mechanisms*. 2nd ed., Pearson, 1997.
2. Ege, Seyhan. *Organic Chemistry: Structure and Reactivity*. 3rd ed., Prentice Hall and Macmillan, 1994.
3. Eliel, Ernest L. *Stereochemistry of Organic Compounds*. John Wiley, 2008.
4. Juaristi, Eusebio. *Introduction to Stereochemistry and Conformational Analysis*. 1st ed., Wiley, 1991.
5. Nasipuri, D. *Stereochemistry of Organic Compounds: Principles and Applications*. 4th ed., New Age International, 2020.
6. Kalsi, P.S. *Stereochemistry, Conformation and Mechanism*. 8th ed., New Age International, 2015.
7. Bruice, Paula Yurkanis. *Organic Chemistry*. 4th ed., Prentice Hall.
8. Clayden, Jonathan, Nick Greeves, Stuart Warren, and Peter Wothers. *Organic Chemistry*. Oxford University Press, 2001.
9. Wade, Leroy G. Jr., Jan William Simek, and M. S. Singh. *Organic Chemistry*. 9th ed., Pearson, 2017.
10. Carey, Francis A., and Richard J. Sundberg. *Advanced Organic Chemistry: Part A, Structure and Mechanism*. Springer, 2007.

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Title of the Course: Physical chemistry - I
Category: Core-theory
Course Code: 24MCHE13T
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide a comprehensive introduction to quantum chemistry, chemical dynamics, thermodynamics, and electrochemistry, focusing on both the physical and mathematical aspects. It covers key theories of quantum mechanics and chemical dynamics, as well as fundamental principles of thermodynamics and electrochemistry, with an emphasis on practical applications. Additionally, students will be introduced to quantum mechanical operators, electrochemical reactions, and the mathematical tools necessary to analyze chemical reactions and systems.

Course Outcomes:
At the end of the course, the student will be able to
1. explain the basic principles of quantum mechanics and solve the Schrödinger equation for model systems.
2. apply reaction rate theories to interpret and calculate the rates of various chemical reactions.
3. analyze thermodynamic properties and equilibria using classical and statistical thermodynamic methods.
4. evaluate the effects of dilution, activity coefficients, and reversible electrochemical cells using electrochemical principles.

Unit 1 Quantum chemistry – I **15**

Introduction to Exact Quantum Mechanical Results. Operator algebra; Eigen values and Eigen functions; operators for momentum and energy; linear combination of Eigen functions of an operator; the Schrodinger wave equation and the postulates of quantum mechanics; discussion of solutions of the Schrodinger equation to some model systems, viz., particle in a box, harmonic oscillator, rigid rotor, hydrogen atom.
Approximate Methods. The variation theorem; perturbation theory (first order and non-degenerate); application of variation method perturbation theory and perturbation theory to the helium atom

Unit 2 Chemical dynamics – I **15**

Theories of Reaction Rates. Collision theory; steric factor; theory of absolute reaction rates-reaction coordinate, activated complex and the transition state; thermodynamic formulation of reaction rates; Arrhenius equation.
Unimolecular Reactions. Lindemann, Lindemann-Hinshelwood, and RRKM theories; termolecular reactions; complex reactions-rate expressions for opposing, parallel and consecutive reaction (all first order type).
Chain Reactions. Dynamic chain; hydrogen-bromine reaction; pyrolysis of acetaldehyde; decomposition of ethane; photochemical reactions-H_2-Br_2, H_2-Cl_2 reactions; autocatalysis; H_2-O_2 reaction; explosion limits; rate expressions for chain reaction

Unit 3 Thermodynamics – I **15**

Brief Review of Thermodynamic Concepts. Enthalpy; entropy; free energy; concept of entropy; entropy as a state function; entropy change in reversible process and irreversible process; temperature-entropy

diagrams; entropy change and phase change; entropy of mixing; entropy and disorder-residual entropy; Maxwell relations.

Classical and Statistical Thermodynamics. Partial molar properties: their significance and determination of partial molar volume, fugacity and its determination; concept of distribution; thermodynamic probability and most probable distribution; ensemble averaging; postulates of ensemble averaging; canonical; grand canonical and micro-canonical ensembles; partition functions; translational, rotational, vibrational and electronic partition functions; Gibbs-Duhem equation; calculation of thermodynamic properties in terms of partition functions; heat capacity; chemical equilibria and equilibrium constant in terms of partition functions; entropy of monatomic gases (Sackur-Tetrade equation)

Unit 4 Electrochemistry – I 15

Strong Electrolytes. Effect of dilution on equivalent conductance-Inter ionic attraction; Debye-Huckel-Onsager treatment; derivation of Debye-Huckel-Onsager equation; verification and limitation of Onsager equation; Bjerrum treatment of electrolytes; Debye-Falkenhagen and Wien effects.

Activity and Activity Coefficients. Relation between different types of activity coefficients; determination of mean ionic activity coefficients by solubility and EMF methods; Debye-Huckel limiting law and its verification (qualitative).

Reversible Electrochemical Cells. Chemical cells and concentration cells; types of reversible electrodes; electrode potentials; reactions in reversible cells; Nernst equation; thermodynamic and kinetic derivation; concentration cells with and without transference; liquid junction potential and its determination; determination of standard potentials; significance of standard half-cell potentials; applications of electrochemical cells; commercial cells; conductometric and potentiometric titrations

Prescribed Textbooks:

1. Atkins, P. W. *Physical Chemistry*. 7th ed., ELBS, 2006.
2. Chandra, A. K. *Introduction to Quantum Chemistry*. 4th ed., Tata McGraw Hill, 2017.

Reference Books:

1. Glasstone, Samuel. *Thermodynamics for Chemists*. 1st ed., Dover Publications, 1960.
2. Klotz, Irving M. *Chemical Thermodynamics*. 1st ed., Addison-Wesley, 1967.
3. Dole, Melvin. *Statistical Thermodynamics*. 1st ed., John Wiley & Sons, 1956.
4. Bockris, John O. M., and A. K. N. Reddy. *Modern Electrochemistry, vol. I & II*. 1st ed., Plenum Press, 1970.
5. Glasstone, Samuel. *An Introduction to Electrochemistry*. 3rd ed., East-West Press, 1968.
6. Levine, Ira N. *Quantum Chemistry*. 7th ed., Prentice Hall, 2013.
7. Chandra, Manas. *Atomic Structure and Chemical Bond*. 1st ed., Springer, 2001.
8. Laidler, K. J. *Chemical Kinetics*. 3rd ed., McGraw Hill, 1987.
9. Rajaraman, J., and Kuriacose, J. *Kinetics and Mechanism of Chemical Transformations*. 2nd ed., Macmillan, 2003.

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Title of the Course: General topics in chemistry
Category: Elective
Course Code: 24MCHE1AT
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide a comprehensive understanding of fundamental concepts in point groups, symmetry, and group theory, alongside a solid foundation in the errors and statistical treatment of analytical data. It offers students the opportunity to explore various chromatographic techniques and their applications, while also delving into the fundamental principles of molecular spectroscopy, including microwave, IR, and Raman spectroscopies, along with the associated rules.

Course Outcomes:
At the end of the course, the student will be able to
1. explain the concepts of symmetry elements and operations, and their application in group theory.
2. apply statistical methods such as the F-test and t-test to analyze experimental data and assess errors.
3. analyze different chromatographic techniques and interpret their principles, instrumentation, and applications.
4. interpret molecular spectra using principles from microwave, infrared, and Raman spectroscopy for molecular structure analysis.

Unit 1 Symmetry and group theory 15

Symmetry elements and symmetry operation; definitions of a group, sub-group; relation between orders of a finite group and its sub-group; conjugacy relation and classes-point symmetry group; Schonflies symbols; representation of groups by matrices (representation for C_{n9} C_{nv9} D_{nh9} etc. groups to be worked out explicitly); character of a representation; the great orthogonality theorem (without proof); character tables and their use in spectroscopy

Unit 2 Errors and statistical treatment 15

Introduction; classification of errors; accuracy; precision; minimization of errors; average; median values; absolute error; relative error; mean deviation; relative mean deviation; standard deviation; relative standard deviation; variance; range; confidence interval; comparison of results: F-test and student's t-test (i. comparison of mean and true value, ii. comparison of two means and iii. comparison of more than two means - ANOVA); Dixon's Q-test; Gaussian distribution of random errors; correlation and regression; significant figures and rules for computations.

Unit 3 Chromatographic techniques 15

Definition and classification; principle, materials, methods and applications of paper chromatography, thin layer chromatography, column chromatography, size exclusion chromatography, ion exchange chromatography; high performance liquid chromatography (HPLC): principle, instrumentation and applications; gas chromatography (GC): principle, instrumentation, GC columns, detectors and applications

Unit 4 Molecular spectroscopy 15

Microwave Spectroscopy. Classification of molecules; rigid rotor model; non-rigid rotor; stark effect.
Infrared Spectroscopy. Review of linear harmonic oscillator; vibrational energies of diatomic molecules; zero-point energy; force constant; bond strengths; anharmonicity; Morse potential energy diagram;

vibration-rotation spectroscopy; PQR branches; vibrations of simple polyatomic molecules (CO_2, H_2O etc.); selection rules; exclusion principle.
Raman Spectroscopy. Classical and quantum theories of Raman effect; pure rotational, vibrational and vibrational-rotational spectra; rotational Raman spectra; selection rules

Prescribed Textbooks:

1. Veera Reddy, K. *Symmetry and Spectroscopy of Molecules*. 1st ed., New Age International Publishers, 2008.
2. Bhattacharya, S. K. *Chemical Applications of Group Theory*. 3rd ed., Wiley India Pvt. Ltd., 2005.

Reference Books:

1. Seader, J. D., and Henley, E. J. *Separation Process Principles*. 3rd ed., John Wiley & Sons Inc, 2011.
2. Berg, E. W. *Physical and Chemical Methods of Separation*. McGraw Hill, 1983.
3. Drago, R. S. *Physical Methods in Chemistry*. Saunders, 1992.
4. Barrow, G. M. *Introduction to Molecular Spectroscopy*. McGraw Hill, 1986.
5. Mendham, J., Denney, R.C., Barnes, J.D., and Thomas, M.J. *Vogel's Textbook of Quantitative Chemical Analysis*. 6th ed., Pearson Education Asia, 2005.
6. Willard, H. W., Merritt, L. L., and Dean, J. A. *Instrumental Methods of Analysis*. 7th ed., Affiliated East-West Press, 1988.
7. Skoog, D. A., and West, D. M. *Principles of Instrumental Analysis*. 4th ed., Holt, Rinehart and Winston, 1992

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Title of the Course: Pharmaceutical quality control and quality assurance
Category: Elective
Course Code: 24MCHE1BT
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide a comprehensive understanding of quality audit fundamentals, including SOP, ICH, and ISO standards. It covers essential documentation processes, material handling, and the roles and responsibilities within pharmaceutical organizations. Additionally, the course imparts knowledge of regulatory aspects, quality control, and the foundational principles of quality assurance, ensuring a well-rounded grasp of industry standards

Course Outcomes:
At the end of the course, the student will be able to
1. understand the principles and guidelines of quality audit, SOP, and international regulations in pharmaceutical industries.
2. apply personnel responsibilities and environmental control measures to maintain hygiene and contamination-free manufacturing environments
3. analyze regulatory aspects and quality control methods in pharmaceutical production and validation processes.
4. evaluate quality assurance principles and management systems to enhance operational quality in chemical industries.

Unit 1 Quality audit documentation and handling 15

Quality audit. Standard operating procedure (SOP); international conference harmonization (ICH); ISO-9000; ISO-14000, WHO specifications, USFDA guidelines and ICMR.
Documentation and Handling: Manufacturing documents, Master Formula, batch formula, Record, Distribution of records, Handling of returned goods, Recovered materials and Reprocessing.

Unit 2 Organization and personnel responsibilities 15

Training, Hygiene, Premises: Location, Design, Plant layout, Construction, Maintenance and Sanitations. Environmental control, Sterile areas, control of contamination

Unit 3 Regulatory aspects and quality control 15

Regulatory aspects. Validation of Personnel, Equipment and cleaning methods, regulatory aspects of pharmaceutics.
Quality Control. In-process quality Control on various dosage forms, Sterile and non- sterile operations

Unit 4 Basic concepts of quality assurance 15

Proton Basic concepts, principles or prescription, Needs, requirements and expectations, characteristics of quality, Achieving, sustaining and improving quality, Quality dimensions and costs of quality.
Elements of quality Assurance, Quality Management System, Quality management concepts and principles: ISO 9001:2000, QMS Case studies on ISO 9001: 2000 in chemical industries.

Prescribed Textbooks:

1. Pannerselvam, R. *Production and Operations Management*. 3rd ed., Prentice Hall India Learning Pvt. Ltd, 2012.
2. Savsar, M. *Quality Assurance and Management*. InTech-Croatia, 2012.

Reference Books:

1. Montgomery, D. C. *Statistical Quality Control*. 5th ed., John Wiley & Sons, 2005.
2. Starr, M. K. *Production and Operations Management*. Biztantra, 2004.
3. Shah, D. H. *QA Manual*. Business Horizons, 2000.
4. Besterfield, D. H., et al. *Total Quality Management*. 3rd ed., Pearson Education, Inc., 2003.
5. Konieczka, P., and J. Namiesnik. *Quality Assurance and Quality Control in the Analytical Chemical Laboratory: A Practical Approach*. 1st ed., CRC Press, 2009.
6. Hoyle, D. *ISO 9000 Quality Systems Handbook*. 5th ed., Butterworth Heinemann-Elsevier, 2006.
7. Prichard, E., and V. Barwick. *Quality Assurance in Analytical Chemistry*. John Wiley & Sons, 2007.

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Title of the Course: Inorganic chemistry practicals
Category: Core practical
Course Code: 24MCHE11L
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	8	4

Course Objectives: The course aims to train students in developing skills for the preparation and processing of inorganic complexes, enhancing their practical abilities in laboratory techniques. Additionally, it provides students with knowledge and hands-on experience in the quantitative analysis of these complexes, fostering a deeper understanding of their properties and applications.

Course Outcomes:
At the end of the course, the student will be able to
1. demonstrate the preparation and purification techniques for various inorganic complexes, ensuring the correct synthesis procedures are followed.
2. analyze the results obtained from the estimation of metal ions in inorganic complexes to assess the accuracy and reliability of the methods used.
3. evaluate the effectiveness of different analytical techniques employed in the estimation of metal ions and propose improvements based on experimental outcomes.

1 Preparation and purification of Inorganic complexes
a) Chloropentammine cobalt(III)chloride
b) Bis(oxalate)cuprate(II) dehydrate
c) Tris(oxalato)ferrate(III)
d) Hexaamminenickel(II) chloride
e) Tetra (ammine) copper (II) sulphate.
f) Tris(acetylacetonato) Manganese (III) chloride
g) Tris(ethylenediammine) nickel(II) thio sulphate

2. Complex analysis
a) Estimation of cobalt present in chloropentammine cobalt(III)chloride
b) Estimation of copper present in bis(oxalate)cuprate(II)dehydrate
c) Estimation of iron present in tris(oxalato)ferrate(III)
d) Estimation of nickel present in hexaamminenickel(II)chloride.
e) Estimation of copper in Tetra (ammine) copper (II) sulphate by titrating with sodium thiosulphate.
f) Estimation of Manganese in Tris(acetylacetonato) Manganese (III) chloride by Volhard's method.
g) Estimation of nickel in Tris(ethylene diammine) nickel (II) thio sulphate by EDTA (Back titration).

Prescribed book:
Mendham, J., Denney, R.C., Barnes, J.D., and Thomas, M.J. *Vogel's Textbook of Quantitative Chemical Analysis*. 6th ed., Pearson Education Asia, 2000.

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Title of the Course: Organic chemistry practicals - I
Category: Core practical
Course Code: 24MCHE12L
Semester: I Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	8	4

Course Objectives: The course aims to provide a comprehensive understanding of the fundamental principles involved in the separation methods of binary mixtures of organic compounds. Additionally, it focuses on the preparation, purification, and identification of organic compounds through single-step synthesis, equipping students with essential skills in organic chemistry techniques.

Course Outcomes:
At the end of the course, the student will be able to
1. demonstrate the ability to select and apply appropriate methods for the separation of a binary mixture of organic compounds.
2. analyze the purity and yield of synthesized organic compounds through recrystallization and melting point determination.
3. evaluate and compare the efficiency of different single-step preparation techniques for the selected organic compounds based on yield and purity outcomes.

Separation of a binary mixture and single step preparation of organic compounds
i) Identification of method of separation of binary mixture of organic compounds.
ii) Single step preparations: Preparation, recrystallization, and determination of melting point & yield of i. nerolin, ii. p-nitro acetanilide, iii. m-dinitrobenzene, iv. phthalimide, v. hippuric acid, vi. 2,3-diphenylquinoxaline, vii. Diels- Alder adduct, viii. Benzotriazole and ix. phenothiazine.

Prescribed book:
Mendham, J., Denney, R.C., Barnes, J.D., and Thomas, M.J. *Vogel's Textbook of Quantitative Chemical Analysis*. 6th ed., Pearson Education Asia, 2000.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Inorganic chemistry - II
Category: Core-theory
Course Code: 24MCHE21T
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide a comprehensive understanding of organometallic chemistry principles and deepen knowledge on the synthesis, properties, structure, and bonding of transition metal π-complexes. Students will be exposed to the analysis of electronic spectra and the magnetic properties of both transition and inner transition metal complexes, enabling them to gain critical insights into these advanced chemical systems.

Course Outcomes:
At the end of the course, the student will be able to
1. explain stoichiometric reactions and catalytic processes in organometallic chemistry, including ziegler-natta polymerization.
2. apply knowledge of transition metal π-complexes to predict their bonding, structure, and reactivity.
3. analyze electronic spectra of transition and inner transition metal complexes using Orgel and Tanabe-Sugano diagrams.
4. evaluate magnetic properties of transition and inner transition metal complexes by analyzing paramagnetism and magnetic exchange.

Unit 1 Organometallic chemistry 15

Stoichiometric reactions in catalysis; homogeneous catalytic hydrogenation; hydroformylation (oxoreaction); isomerization; Zeigler-Natta polymerization of olefins; oxopalladation reactions; activation of small molecules by coordination; fluxionality and dynamic equilibria in compounds such as η^2-olefin, η^3-allyl and dienyl complexes.

Unit 2 Transition metal π-complexes 15

Transition metal π-complexes with unsaturated organic molecules such as alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, general methods of preparation, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on ligands

Unit 3 Electronic spectra of transition & inner transition metal complexes 15

Free Ion terms and energy levels: configurations, terms, states and microstates; calculation of microstates for p^2 and d^2 configuration; L-S (Russell-Saunders) coupling schemes; J-J coupling scheme; derivation of terms for p^2 and d^2 configuration; hole formulation; energy ordering of terms (Hund's Rules); Selection rules: Laporte orbital selection rule, spin selection rules; splitting of energy levels and spectroscopic states, Orgel diagrams of d^1 to d^9 metal complexes; interpretation of electronic spectra of aquo complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II); calculation of interelectronic and spectra parameters for d^8 metal complexes; Tanabe-Sugano diagrams for d^2 and d^6 octahedral complexes; charge transfer (L → M and M → L) spectra of metal complexes. Spectral properties of inner transition metal complexes (lanthanides and actinides)

Unit 4 Magnetic properties of transition & inner transition metal complexes 15

Diamagnetism; paramagnetism; orbital and spin contributions; spin-orbit coupling; Hund's third rule and energies of J levels; Curie law and Curie-Weiss law; ferromagnetism and antiferromagnetism; temperature independent magnetism; magnetic susceptibility and determination of magnetic susceptibility by Gouy method; paramagnetism and crystalline fields – Ti^{3+}, V^{3+}, VO^{2+}, Cr^{3+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+} and Cu^{2+}; magnetic exchange in copper acetate and other dimers. Magnetic properties of inner transition metal complexes (lanthanides and actinides)

Prescribed Textbooks:

1. Cotton, F. A., Wilkinson, G., Bochmann, M., and Grimes, R. N. *Advanced Inorganic Chemistry*. 5th ed., John Wiley & Sons Inc., 1988.
2. Huheey, J. E., Keiter, E. A., and Keiter, R. L. *Inorganic Chemistry: Principles of Structure and Reactivity*. 4th ed., Prentice Hall, 1993.

Reference Books:

1. Kettle, S. F. *Coordination Compounds*. Springer, 1975.
2. Carlin, R. L. *Magnetochemistry*. Springer-Verlag New York, 1986.
3. Dutta, R. L., and Syamal, A. *Elements of Magnetochemistry*. 2nd ed., Affiliated East-West Press Pvt. Ltd., 1993.
4. Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*. 4th ed., Wiley Interscience, 2005.
5. Mehrotra, R. C., and Singh, A. *Organometallic Chemistry: A Unified Approach*. 2nd ed., New Age International, 2006.
6. Powell, P. *Principles of Organometallic Chemistry*. 2nd ed., ELBS, 1988.
7. Wulfsberg, G. *Inorganic Chemistry*. University Science Books, 2000.
8. Figgis, B. N. *Introduction to Ligand Fields*. Krieger Pub Co., 1976.
9. Lee, J. D. *Concise Inorganic Chemistry*. 5th ed., Wiley-Blackwell, 1996.
10. Jolly, W. L. *Modern Inorganic Chemistry*. 2nd ed., McGraw-Hill, 1991.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Organic chemistry - II
Category: Core-theory
Course Code: 24MCHE22T
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide a comprehensive understanding of various chemical reaction mechanisms, including electrophilic, nucleophilic, and free radical addition reactions, as well as condensation reactions through name reactions. Students will gain insights into elimination, esterification, and hydrolysis mechanisms, along with the mechanisms and applications of molecular rearrangement reactions. Additionally, the course will cover systematic nomenclature and the aromatic behavior of heterocyclic compounds.

Course Outcomes:
At the end of the course, the student will be able to
1. explain the mechanisms and stereospecificity of electrophilic and nucleophilic addition reactions.
2. apply the concepts of elimination, esterification, and hydrolysis reactions to predict their outcomes.
3. analyze different molecular rearrangements and their mechanisms in organic chemistry.
4. evaluate the nomenclature and aromaticity criteria of heterocycles in relation to structural features.

Unit 1 Addition reactions 15

Introduction. electrophilic additions (Br_2, HBr, HOBr, and H_2O/H_2SO_4); Markovnikov's rule, free radical addition-Kharash peroxide effect (Anti-Markovnikov rule), nucleophilic additions (Aldol, Cannizaro, Michael, Robinson annulation, Baylis-Hilman Reaction, Darzens condensation, Mannich, Claisen, Dieckmann, Perkin, Knoevenagel, Claisen-Schmidt, Benzoin and Stobbe condensation reactions, Grignard and Wittig reactions).
Stereospecificity in addition reactions: bromination, dihydroxylation, hydroboration, hydrogenation (heterogenous) and epoxidation reactions

Unit 2 Elimination, esterification and hydrolysis reactions 15

Elimination Reactions. Introduction; type of eliminations: α-, β- and γ-eliminations; Zaitsev (Saytzeff) and Hofmann rules; mechanism: E1, E2 and E1cB; competition between elimination and substitution; stereochemistry and orientation in E2 eliminations; pyrolytic syn elimination; dehydration of alcohols; dihydro-eliminations of C-C, C-O and C-N; dihalo-elimination; decarboxylative eliminations; molecular rearrangement during elimination; fragmentation reactions.
Esterification Reactions. Reaction between carboxylic acid and alcohol: Fischer, Mitsunobu and Steglich esterifications; reaction between acid halide and alcohols; reaction between carboxylic acid and alkyl halides; trans esterification.
Hydrolysis Reactions. General mechanism and applications of ester hydrolysis in acidic and basic conditions; hydrolysis of acid halides; hydrolysis of amides

Unit 3 Molecular rearrangements 15

Introduction; types of molecular rearrangements; migratory aptitude; rearrangements to electron deficient carbon: pinacol-pinacolone, Wagner-Meerwein, Wolff, benzil-benzilic acid and Demjanov rearrangements; rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements; rearrangements to electron deficient oxygen: Baeyer-Villiger and Dakin

rearrangements; rearrangements to electron rich carbon: Favorskii and Neber; rearrangements to aromatic ring: thermal Fries, benzidine and Hofmann-Martius rearrangements.

Unit 4 Nomenclature and aromaticity of heterocycles 15

Nomenclature of Heterocycles. Systematic nomenclature (Hantzsch-Widman system); trivial system; fusion nomenclature system; replacement nomenclature system; monocyclic heterocycles, fused heterocycles, spiroheterocycles; bridged heterocycles; bicyclic systems; polycyclic systems; heterocyclic ring assemblies.

Aromaticity of Heterocycles. Chemical behavior of aromatic heterocycles; five and six-membered aromatic heterocycles and mixed aromatic heterocycles; relationship with carbocyclic aromatic compounds; criteria of aromaticity in heterocycles; structural and electronic criteria.

Prescribed Textbooks:

1. Smith, Michael B., and Jerry March. *Advanced Organic Chemistry-Reactions, Mechanism, and Structure.* 6th ed., John Wiley & Sons, 2007.
2. Carey, Francis A. *Organic Chemistry.* 4th ed., McGraw-Hill Higher Education, 2000.

Reference Books:

1. Carey, Francis A., and Richard J. Sundberg. *Advanced Organic Chemistry, Part B, Reactions and Synthesis.* 5th ed., Springer, 2008.
2. Kurti, Laszlo, and Barbara Czako. *Strategic Applications of Named Reactions in Organic Synthesis.* Elsevier, 2005.
3. Sykes, Peter. *A Guide Book to Mechanism in Organic Chemistry.* 6th ed., Longman and Wiley, 1986.
4. Gupta, R. R., M. Kumar, and V. Gupta. *Heterocyclic Chemistry Vol. 1-3.* Springer Verlag, 1998.
5. Joule, J. A., and Keith Mills. *Heterocyclic Chemistry.* 5th ed., Wiley, 2010.
6. Quin, Louis D., and John A. Tyrell. *Fundamentals of Heterocyclic Chemistry.* Wiley, 2010.
7. Bruice, Paula Yurkanis. *Organic Chemistry.* 4th ed., Prentice Hall, 2003.
8. Clayden, Jonathan, Nick Greeves, Stuart Warren, and Peter Wothers. *Organic Chemistry.* Oxford University Press, 2001.
9. Wade, Leroy G. Jr., Jan William Simek, and M. S. Singh. *Organic Chemistry.* 9th ed., Pearson, 2017.
10. Carey, Francis A., and Richard J. Sundberg. *Advanced Organic Chemistry, Part A, Structure and Mechanism.* 5th ed., Springer, 2007.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Physical chemistry - II
Category: Core-theory
Course Code: 24MCHE23T
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to explore the practical applications of quantum chemistry, chemical dynamics, thermodynamics, and electrochemistry. It includes an in-depth study of quantum mechanical theories related to angular momentum and conjugated systems, as well as the principles of catalysis and the laws of both classical and statistical thermodynamics. Additionally, students will gain expertise in interpreting key physical quantities in thermodynamics, understanding the Debye-Hückel Limiting Law, and applying electrochemical theories to analyze electrode kinetics.

Course Outcomes:
At the end of the course, the student will be able to
1. explain angular momentum concepts and molecular orbital theory, applying the Pauli Exclusion Principle and Hückel theory to molecular systems.
2. apply mechanisms of acid-base catalysis and homogeneous and heterogeneous catalysis in various chemical reactions.
3. analyze phase equilibria and the phase rule using the Clausius Clapeyron equation in different systems.
4. investigate electrochemical techniques and fuel cell technologies, identifying their applications and limitations.

Unit 1 Quantum chemistry – II **15**

Angular momentum. Angular momentum; rotations and angular momentum; Eigen functions and Eigen values of angular momentum; ladder operator; addition of angular momenta; spin angular momenta; anti-symmetry and Pauli Exclusion Principle; Slater determinant.
Molecular Orbital Theory. Hückel theory of conjugated systems; π-bond order and charge density calculations; application to ethylene, butadiene and benzene; molecular term symbols; Russell– Saunders coupling

Unit 2 Chemical dynamics – II **15**

Acid Base Catalysis. Specific acid catalysis and general acid catalysis (hydrolysis of ester and vinyl ether); specific base catalysis and general base catalysis (the alcohol reaction and hydrolysis of acetic anhydride); protolytic and prototropic mechanism.
Homogeneous and Heterogeneous Catalysis. Homogeneous catalysis; catalysis by transition metal ions and their complexes; industrially important processes; supported transition metal complexes as catalysts; bimolecular reactions; electronic theories of chemisorption and heterogeneous catalysis.
Introduction to Enzyme Catalysis. Michaeles - Menton Kinetics - Effect of pH and effect of temperature on the rates of enzyme reactions

Unit 3 Thermodynamics – II **15**

Phase Equilibria. Equilibrium between two phases of one component; the Clapeyron equation; the Clausius Clapeyron equation, applications; integrated form of Clapeyron equation.
Phase rule. Thermodynamic derivation of phase rule; solid-liquid equilibria; thermal analysis; simple eutectic, congruent fusion, incongruent, fusion and systems consisting of both; application of phase rule

to three component system; Stokes and Roozeboom plots; three component liquid systems; formation of one pair, two pairs and three pairs of partially miscible liquids; two salts and water; no chemical combination; double salt formation; one salt forms hydrate and two salts form hydrates; solid solutions

Unit 4 Electrochemistry – II 15

(A) Batteries: Primary and secondary batteries. Fuel cells: Hydrogen-Oxygen Fuel cells. Methanol-Oxygen Fuel cells. Proton exchange membrane fuel cells-Advantage and limitations of fuel cells. UPS and its working principles & applications.

(B) Electrochemical study: Potentiometry: Types of electrodes (Hydrogen, Calomel and Glass). Mass transport by migration, convection and diffusion. Electrochemical synthesis of solid materials. Solid state electrochemistry. Ion conducting polymers, electronically conducting polymers and redox polymers. The electrochemical double layer. D.C. Polarography: Dropping mercury electrode, Application and instrumentation of polarography. Potentiostatic and galvanostatic methods including chronoamperometry and cyclic voltammetry, Applications of cyclic voltammetry. Types of corrosion and corrosion protection. Electroplating.

Prescribed Textbooks:

1. Atkins, P. W. *Physical Chemistry*. 5th ed., ELBS, 1994.
2. Chandra, A. K. *Introduction to Quantum Chemistry*. 4th ed., Tata McGraw Hill, 1994.

Reference Books:

1. Glasstone, Samuel. *An Introduction to Electrochemistry*. 3rd ed., Affiliated East-West, 1960.
2. Moroi, Yoshikiyo. *Micelles: Theoretical and Applied Aspects*. Plenum Press, 1992.
3. Glasstone, Samuel. *A Textbook of Physical Chemistry*. 2nd ed., Macmillan, 1946.
4. Maron, Samuel H., and Carl F. Prutton. *Principles of Physical Chemistry*. 4th ed., Macmillan, 1965.
5. Antropov, L. I. *Theoretical Electrochemistry*. Mir Publishers, 1972.
6. Levine, Ira N. *Quantum Chemistry*. 6th ed., Prentice Hall, 2009.
7. Mcweeny, R. *Coulson's Valence*. 3rd ed., ELBS, 1979.
8. Bockris, J. O. M., and A. K. N. Reddy. *Modern Electrochemistry*, Vol. I & II. 2nd ed., Plenum, 1998.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Applied and environmental aspects
Category: Elective
Course Code: 24MCHE2AT
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: This course aims to provide comprehensive knowledge and hands-on experience in various analytical techniques. Students will gain expertise in the preparation of sampling, decomposition, separation, and preconcentration methods. The course also covers the analysis of fertilizers, pesticides, minerals, ores, fuels, alloys, and explosives, while emphasizing water quality monitoring.

Course Outcomes:
At the end of the course, the student will be able to
1. demonstrate the ability to prepare analytical samples by applying appropriate sampling techniques and understanding sampling uncertainties.
2. analyze and interpret soil and fertilizer samples using techniques such as gas chromatography and spectrophotometry to determine nutrient and contaminant levels.
3. evaluate the properties and composition of various fuels and alloys through systematic analysis and characterization methods.
4. design and implement water and air quality monitoring plans that utilize analytical methods to assess the presence of pollutants and their impact on the environment.

Unit 1 Sampling and separation methods 15

Preparing the sample for analysis: Sampling, The effect of sampling uncertainties, Gross sample, determination of the size of the gross sample. Analytical sample. Preparation of laboratory sample from gross sample, Moisture in the sample, Karl-Fisher reagent for the determination of moisture content in samples.
Decomposition and dissolving the sample: Decomposition of sample by fluxes, wet digestion, dry ashing, combustion with oxygen, microwave decomposition.
Separation and pre-concentration: Extractive separation of metal ions as chelates (dithizone, oxine, APDC, NaDDTC), Solid-phase extraction

Unit 2 Analysis of agro chemicals and minerals 15

Soil analysis: Soil moisture, pH, total nitrogen, Phosphorus, silica, boron and metals (Cd, Cu, Fe, Mn, and zinc) in soil.
Fertilizer analysis: Analysis of Ammonical fertilizers, Phosphate fertilizers, Nitrate fertilizers Pesticide Analysis: Analysis of organo chlorine pesticides by gas chromatography, Determination of DDT residue in vegetable and food grains. Analysis of organo phosphorous pesticides (Malathion, parathion) by spectrophotometric and chromatographic methods.
Analysis of Minerals and Ores: Limestone, Ilmenite, Chalcopylites and Beryl. Analysis of Cement, Ceramics and glass

Unit 3 Analysis of complex materials 15

Analysis of Fuels: Coal, proximate and ultimate analysis, heating valves and grading of coal. Liquid Fuels: Flash point, aniline point, octane number and carbon residue.
Analysis of Gaseous Fuels: Producer gas, Water gas, Calorific values

Analysis of alloys: German Silver, Brass, bronze, Solder, Steels containing elements such as Mo, Co, Cr, Ni. Aanalysis of Explosives: Introduction, Classification, Deflagrating or low explosives, Characteristics of explosives, Nitrocellulose, PETN or PENTHRIT, Di-nitrobenzene (DNB), Trinitrobenzene (TNB), Trinitrotoluene (TNT)

Unit 4 Environmental pollution monitoring 15

Water Quality monitoring: Methods of water sample collection, Determination of Dissolved oxygen (D.O), Biochemical Oxygen Demand (BOD) and Chemical Oxygen Demand(COD)
Analytical methods for the determination of the following ions in water.
Anions: F-, PO4 Cations: Cr, As, Pb, Hg, Cd
Air Quality Monitoring: Air sampling methods, Chemical analysis of the following Air pollutants.
i) Gaseous pollutants: Carbon monoxide (CO). sulphur dioxide (SO_2), nitrogen dioxide (NO_2), Aliphatic hydrocarbons and polycyclic aromatic hydrocarbons (PAH). (ii) Particulate matter

Prescribed Textbooks:

1. Christian, Gary D., John Lalily, and Senes. *Analytical Chemistry*. 6th ed., New York, 2007.
2. Skoog, Douglas A., Donald M. West, and James F. Holler. *Fundamentals of Analytical Chemistry*. 7th ed., Thomson Brooks/Cole, 2001.

Reference Books:

1. Black, C.A. *Methods of Soil Analysis: Part I and II*. American Society of Agronomy.
2. Harrison, John. *Handbook of Analytical Control of Iron and Steel Production*. Wiley, 1979.
3. Welcher, Frank J. *Standard Methods of Chemical Analysis*. D. Van Nostrand Company.
4. Griffin, R.C. *Technical Methods of Analysis*. McGraw-Hill.
5. De, Anil Kumar. *Environmental Chemistry*. Wiley Eastern Ltd.
6. Harge, I.G. *Analytical Chemistry: Principles and Techniques*. Prentice Hall.
7. Skoog, Douglas A., and James J. Loacy. *Principles of Instrumental Analysis*. W.B. Saunders.
8. Strem, A.C., and others. *Fundamentals of Air Pollution*. Academic Press, 1975.
9. American Public Health Association. *Standard Methods for the Examination of Water and Waste Water*. 15th ed., 1981.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Chemistry in day-to-day life
Category: Elective
Course Code: 24MCHE2BT
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
4	-	-	4

Course Objectives: The course aims to provide students with a comprehensive understanding of fundamental chemistry concepts relevant to everyday life. It will cover the composition and role of soil nutrients and food additives, as well as the chemical properties of soaps, detergents, and disinfectants. This knowledge will equip students with practical insights into how chemistry impacts various aspects of daily living.

Course Outcomes:
At the end of the course, the student will be able to
1. identify and classify the structures and biological roles of carbohydrates, proteins, lipids, nucleic acids, and vitamins in human health.
2. analyze the functions of essential plant nutrients and the impact of fertilizers and food additives on soil fertility and food safety.
3. evaluate the synthesis and applications of various dyes and pigments, focusing on their chemical properties and industrial uses.
4. assess the composition and analysis techniques of natural fats, oils, soaps, and detergents to determine their effectiveness and environmental impact.

Unit 1 Essential micronutrients 15

Carbohydrates, proteins, lipids, nucleic acids and vitamins: definition, sources, classification, applications and diseases due to deficiency.

Classification of amino acid- structure, essential and non essential amino acids, zwitter ion, isoelectric point, amphoteric property, Peptide bond. biological roles of protein. Classification of proteins according to shape, composition and solubility Structure of protein, chemical bonds involved in protein structure. Physical-chemical properties of proteins. Classification of lipids according to chemical composition, fatty acids; saturated and unsaturated fatty acids. Fatty acids-essential fatty acids, structure, chemical reactions of lipids: Reactions involving COOH group, Reactions involving double bond, reaction involving OH groups.

Unit 2 Soil nutrients and food additives 15

Plant nutrients, nutrient function, micronutrients, need for fertilizers, fertility and pH of the soil, Fertilizers - classification, characteristics and uses, pesticides and insecticides: definition, classification, characteristics and uses; additives: definition, characteristics, uses and abuse of additives in foods and beverages

Unit 3 Dyes, paints and pigments 15

Fundamental of dyes: General, Important chemical chromophores of dyes, Dyes Class for principle applications, Description of individual of class and synthesis of some commercial dyes. Dyes for electro optical application: Molecular Orbital design, Synthesis and characteristics of functional dyes. Near infrared absorption (NIR) dyes: Introduction, Cyanine type chromophores, donar-acceptor chomophores, applications. Colorants for high technology, Color and constitution relationships in Azoacetoacetanilide

pigments. Organic Pigments: Synthesis, Characterizam and application. Some other aspects related to dyes: Non matagenic dyes, colourants for high technology Fluorescent Brightening agents.

Unit 4 Soaps and detergents 15

Introduction to natural fats and oils, Analysis of oils and fats: Softening point, Congent point, Titre point, cloud point, Iodine, Saponification, acid, hydroxyl, R-M and Polenskevalue, Elaiden test.

Introduction to soaps, analysis of soap (saponifiable, unsaponifiable) and for unsaponified matter in soaps, Estimation of free alkali and phenol in soap. Classification of detergents (in Brief): Analysis of active ingredients from detergents (methylene blue and Hyamine-1622 method); Estimation of CMC, Chlorides, total phosphates etc.

Prescribed Textbooks:

1. Sharma, B.K. *Industrial Chemistry*. 9th ed., Goel Publishing House, 2005.
2. Bagavathi Sundari, K. *Applied Chemistry*. M.J.P. Publishers, 2006.
3. Connell, Des W. *Basic Concepts of Environmental Chemistry*. 2nd ed., Taylor & Francis Group, 2016.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Organic chemistry practicals - II
Category: Core practical
Course Code: 24MCHE22L
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	8	4

Course Objectives: The course aims to provide a comprehensive understanding of the techniques and principles involved in the isolation and identification of natural products. It covers the methodologies for isolating these compounds, as well as the various methods for their identification. Additionally, the course focuses on the principles underlying the estimation of organic compounds, equipping students with essential skills for practical applications in the field.

Course Outcomes:
At the end of the course, the student will be able to
1. apply extraction techniques to isolate and identify natural products from various sources.
2. analyze the chemical properties of isolated compounds through estimation methods.
3. evaluate the significance of natural products in pharmaceuticals by comparing estimation results with standard reference values

1 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 powder
   d) Isolation of piperine from black pepper
   e) Isolation of lycopene from tomatoes
   f) Isolation of hesperidin from orange peel

2. Estimations of organic compounds
   a) Estimation of glucose
   b) Estimation of aspirin
   c) Estimation of paracetamol
   d) Estimation of ibubrofen

Prescribed Textbooks:

1. Vogel, A.I. *Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis*. 5th Ed., Longman, 1989.
2. Ikan, R. *Natural Products: A Laboratory Guide*. 2nd Ed., Academic Press, 1991.
3. Sethi, P.D. *Quantitative Analysis of Drugs in Pharmaceutical Formulations*. 1st Ed., CBS Publishers & Distributors, 1996.
4. Mann, F.G., and Saunders, B.C. *Practical Organic Chemistry*. 4th Ed., Pearson Education, 2009.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Physical chemistry practicals
Category: Core practical
Course Code: 24MCHE23L
Semester: II Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	8	4

Course Objectives: The course aims to provide comprehensive training in the operation of various analytical instruments used for analyzing chemical constituents

Course Outcomes:
At the end of the course, the student will be able to
1. apply conductometric and potentiometric techniques to determine dissociation constants and analyze titration curves for acid-base reactions.
2. analyze the effects of electrolyte concentration on the critical solution temperature in the phenol-water system.
3. evaluate experimental data to derive the rate constant for acid hydrolysis of an ester, discussing the influence of catalyst concentration and temperature.

List of experiments
1. Determination of critical solution temperature of phenol-water system and study the effect of electrolyte on CST.
2. Determination of eutectic composition and temperature of simple eutectic system (Urea-benzoic acid).
3. Determination of congruent composition and temperature of binary system (diphenylamine – benzophenone system)
4. Determination of rate constant of acid hydrolysis of an ester and investigate the effect of catalyst concentration, reactant concentration and temperature.
5. Conductometry
   i) Determination of cell constant.
   ii) Verification of Onsager equation.
   iii) Determination of dissociation constant of a weak acid.
   iv) Titration of a strong acid with a strong base.
   v) Titration of a weak acid with a strong base.
6. Potentiometry
   i) Titration of a strong acid with a strong base
   ii) Titration of a weak acid with a strong base
   iii) Titration of ferrous ammonium sulphate with potassium dichromate.

Prescribed book:
Kitchener, J.A. *Findlay's Practical Physical Chemistry*. 8th ed., Longmans, 1978.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Inorganic Chemistry – III
Category: M.Sc.
Couse Code: 24MCHE31T
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: his course aims to provide students with a comprehensive understanding of ESR and Mössbauer Spectroscopy and their relevance in chemical analysis. It introduces the structure and function of metalloproteins involved in dioxygen transport and electron transfer. The course also covers the principles, instrumentation, and applications of Photoelectron Spectroscopy (PES). Additionally, it imparts essential knowledge on the synthesis and characterization of nanomaterials.

Course Outcomes:
At the end of the course, the student will be able to
1. explain the principles and applications of ESR and Mössbauer spectroscopy in identifying structural and bonding features of metal complexes.
2. apply bioinorganic chemistry concepts to describe the role of metal complexes in oxygen transport and biological electron transfer processes.
3. analyze spectroscopic data obtained from photoelectron spectroscopy to interpret chemical structures and bonding.
4. evaluate various chemical synthesis methods and characterization tools for designing and analyzing nanomaterials.

Unit 1 Electron Spin Resonance and Mössbauer Spectroscopy 15

Electron Spin Resonance Spectroscopy. Introduction; principle; instrumentation; selection rules; g- factor and its significance; hyperfine and super hyperfine coupling; zero-field splitting including Kramer's degeneracy; application of ESR to free radicals and transition metal complexes; evidence for covalence in complexes ex. Cu(II)bissalicylaldimine, bis-acetylacetanatovanadyl and hexachloroiridium(IV) complexes.
Mössbauer Spectroscopy. Basic principles; isomer shift; quadrupole shift and spectrum display; applications: bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin and Sn^{2+} and Sn^{4+} compounds, nature of metal-ligand bond, coordination number, unequivalent mössbauer atoms

Unit 2 Bioinorganic Chemistry 15

Transport and Storage of Dioxygen. Metal complexes as oxygen carriers; heme proteins – structure and functions of hemoglobin and myoglobin; non-heme proteins – hemoerythrin and hemocyanin; model synthetic complexes of iron; cobalt and copper
Electron Transfer in Biology. Structure and functions of metalloproteins in electron transfer process; catalase; peroxidase; cytochromes and iron-sulfur proteins; synthetic models

Unit 3 Photoelectron Spectroscopy 15

Photoelectric effect; Koopmans theorem ionization energy; block diagram of photoelectron spectrometer: sources of radiation, monochromator, detectors, shake-up and shake-off features; Ultravoilet photoelectron spectroscopy; application of UPS to O_2 and N_2 molecules; electron spectroscopy of chemical analysis; applications of XPES to qualitative analysis; chemical shift; application to surface studies and structural analysis

Unit 4 Introduction to Nanomaterials 15

Basic chemistry for nanoscience, chemical routes for synthesis of nanomaterials: chemical precipitation and co-precipitation, metal nanocrystals by reduction, sol-gel synthesis, microemulsions or reverse micelles, solvothermal synthesis, microwave heating synthesis, sonochemical synthesis, top down approach of nanomaterials' synthesis. Characterization of nanomaterials: X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM). Applications of nanomaterials in health, energy, and environment

Prescribed books:

1. Willard, Hobart H., Merritt, Lynne L., and Dean, John A. *Instrumental Methods of Analysis*. 7th ed., Wadsworth Publishing (Van Nostrand), 1988.
2. Cotton, F. Albert, Wilkinson, Geoffrey, Bochmann, Manfred, and Grimes, Robert N. *Advanced Inorganic Chemistry: A Comprehensive Text*. 6th ed., Wiley-Interscience, 1999.

Reference Books:

1. Jolly, William L. *Modern Inorganic Chemistry*. Revised ed. (International Student Edition), McGraw-Hill, 1984.
2. Ghosh, Pradip K. *Introduction to Photoelectron Spectroscopy*. Rev. ed., Wiley/Interscience, 1983.
3. Ozin, Geoffrey A., Arsenault, André C., and Cademartiri, Ludovico. *Nanochemistry: A Chemical Approach to Nanomaterials*. 2nd ed., Royal Society of Chemistry, 2009.
4. Ajayan, Pulickel M., Schadler, Linda S., and Braun, Paul V. *Nanocomposite Science and Technology*. 1st ed., Wiley-VCH, 2003.
5. Wang, Zhong Lin, editor. *Characterization of Nanophase Materials*. 1st ed., Wiley-VCH, 2000.
6. Huheey, James E., Keiter, Ellen A., and Keiter, Richard L. *Inorganic Chemistry: Principles of Structure and Reactivity*. 5th ed., Pearson Education, 2022.
7. Wulfsberg, Gary. *Foundations of Inorganic Chemistry*. 1st ed., University Science Books, 2017.
8. Lee, J. Derek. *Concise Inorganic Chemistry*. 5th ed., Wiley-Blackwell, 2008.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Organic Chemistry – III
Category: M.Sc.
Couse Code: 24MCHE32T
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course equips students with the ability to analyze pericyclic reactions using molecular orbital symmetry principles. It offers a detailed understanding of photochemical reaction mechanisms through named reactions. Emphasis is also placed on green chemistry concepts and environmentally friendly synthetic techniques. Furthermore, the course explores the synthesis and medicinal relevance of heterocyclic compounds containing nitrogen, oxygen, and sulfur.

Course Outcomes:
At the end of the course, the student will be able to
1. analyze pericyclic reactions using molecular orbital symmetry and selection rules to predict reaction pathways.
2. apply photochemical principles to predict and explain the mechanisms of various organic photoreactions.
3. explain the principles and synthetic applications of green chemistry techniques in organic synthesis.
4. evaluate the reactivity and medicinal potential of heterocyclic compounds containing nitrogen, oxygen, and sulfur.

Unit 1 Pericyclic Reactions 15

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system and 2,4-pentadienyl systems; classification of pericyclic reactions; electrocyclic reactions: conrotatory and disrotatory motions in 4n, 4n+2 systems; cycloadditions: antarafacial and suprafacial additions in 4n (2+2 cyclo addition) and 4n+2 (4+2 cyclo addition) systems, 1,3-dipolar cycloadditions and cheleotropicreactions; sigmatropic rearrangements: 1,3 and 1,5 suprafacial and antarafacial shifts of H and C, Claisen, Cope and oxy-Cope rearrangements; Ene reaction; FMO and PMO approach; Woodward-Hoffmann correlation diagrams and Woodward-Hoffmann selection rules of electrocyclic reactions, cyclo addition reactions and sigmatropic rearrangements

Unit 2 Photochemistry 15

Photochemical energy; Jablonski diagram; singlet and triplet states; photosensitization; quantum yield; photochemistry of carbonyl compounds: Norrish type-I and Norrish type-II cleavages; Paternò-Büchi reactions; photoreduction; Rearrangement of cyclohexenones, cyclohexadienones; photochemistry of 1,3-butadienes, di-π-methane rearrangement, oxa-di-π-methane rearrangement; photoisomerization of benzene, photo-Fries rearrangement of phenyl esters and anilides; Barton reaction

Unit 3 Green Chemistry 15

Concept of green chemistry, constituent principles of green chemistry, green synthetic methods – organic reactions in aqueous media: advantages and applications in pinacol coupling, Mukaiyama-aldol reaction, and Trost-Tsuji reaction; ionic liquids in organic synthesis: introduction, composition, and application in stereoselective halogenation, Friedel-Craft reaction and hydroformylation; microwave assisted reactions:

principle, conditions, advantages over conventional heating, and application in Fischer-indole synthesis, Paal-Knorr pyrrole synthesis, Baylis-Hillman and benzil-benzilicacid rearrangement; phase transfer catalysis: introduction, types of phase transfer catalysts, mechanism of catalytic action, and application in benzoin condensation, Wittig, Wittig-Horner and Michael addition reactions; ultrasound assisted synthesis: introduction, advantages, applications in the synthesis of Diels- Alder, hydroboration and Reformatsky reactions

Unit 4 Nitrogen, Oxygen and Sulphur Based Heterocycles 15

Synthesis, chemical reactivity, and medicinal importance of heterocycles such as pyrazoles (e.g., Celecoxib), imidazoles (e.g., Metronidazole), oxazoles (e.g., Oxaprozin), isoxazoles (e.g., Leflunomide), thiazoles (e.g., Thiamine), benzopyrroles (e.g., Indomethacin), benzofurans (e.g., Amiodarone), benzothiophenes (e.g., Raloxifene), quinolines (e.g., Chloroquine), and isoquinolines (e.g., Papaverine), with emphasis on their roles in drug molecules.

Prescribed books:

1. Carey, Francis A., and Sundberg, Richard J. *Advanced Organic Chemistry: Part A: Structure and Mechanisms*. 6th ed., Springer, 2013.
2. Carey, Francis A., and Sundberg, Richard J. *Advanced Organic Chemistry: Part B: Reactions and Synthesis*. 6th ed., Springer, 2013.

Reference Books:

1. March, Jerry, and Smith, Michael B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. 7th ed., Wiley-Interscience, 2013.
2. Rohatgi-Mukherjee, K. K. *Fundamentals of Photochemistry*. Revised ed. (1st), Wiley, 1978.
3. Gilbert, Andrew, and Baggott, James E. *Essentials of Molecular Photochemistry*. 1st ed., Blackwell Scientific Publications, 1991.
4. Coyle, John D. *Introduction to Organic Photochemistry*. 1st ed., Wiley, 1986.
5. Griesbeck, Axel G., and Mattay, Jochen, editors. *Synthetic Organic Photochemistry*. 1st ed., Marcel Dekker, 2005.
6. Lancaster, Mike. *Green Chemistry: An Introductory Text*. 3rd ed., Royal Society of Chemistry, 2016.
7. Ahluwalia, V. K., and Aggarwal, Renu. *Organic Synthesis: Special Techniques*. 2nd ed., Alpha Science, 2006.
8. Li, Chao-Jun. "*Organic Reactions in Aqueous Media with a Focus on Carbon–Carbon Bond Formations: A Decade Update*." Chemical Reviews, vol. 105, no. 8, 2005, pp. 3095–3165.
9. Gilchrist, Thomas L. *Heterocyclic Chemistry*. 4th ed., Wiley, 2010.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Physical Chemistry-III
Category: M.Sc.
Couse Code: 24MCHE33T
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course provides foundational knowledge of surface chemistry, including adsorption and thermodynamics at interfaces. It develops a clear understanding of polymers, covering their classification, synthesis, and molecular weight determination. Students gain insights into structural characterization techniques using X-ray diffraction and fluorescence. The course also introduces nuclear chemistry and its applications in analytical, industrial, and pharmaceutical contexts.

Course Outcomes:
At the end of the course, the student will be able to
1. analyze adsorption behavior of molecules at interfaces using Gibbs, Langmuir, and BET isotherms.
2. apply methods to determine polymer molecular weights and classify polymerization processes.
3. explain the working principles and applications of X-ray diffraction and fluorescence techniques in material analysis.
4. evaluate nuclear techniques and instruments used in radiochemical analysis and pharmaceutical applications.

Unit 1 Surface Chemistry 15

Structural and theoretical treatment of liquid interfaces; thermodynamics of binary system; Gibbs equation and verification of Gibbs equation by microtome method and tracer method; spreading of one liquid on anther; states of monomolecular films; the surface area of solids; mixed films; Gibbs adsorption isotherm; the Longmuir adsorption isotherm; BET adsorption isotherm; estimation of surface area (BET equation, theoretical concept); adsorption time; Non equilibrium thermodynamics (entropy production in irreversible process); membrane transport in biochemical reactions

Unit 2 Polymers-Basics and Characterization 15

Basic Concepts. Monomers; repeating units; degree of polymerization; linear, branched and network polymers; classification of polymers.
Polymerization Methods. Condensation, addition, (radical, chain, ionic & coordination) copolymerization, controlled free radical polymerization, viz. NMP, ATRP, and RAFT.
Average Molecular Weight Concepts. Number; weight and viscosity average molecular weights; dispersity - molecular weight distribution; measurement of molar mass of the polymer: end group, viscosity, light scattering, osmotic and ultracentrifugation methods. Measurement of average molecular molar mass of polymers, Gel Permeation Chromatography (GPC)

Unit 3 X-Ray Techniques 15

Phase X-ray Diffraction. Bragg conditions; Miller Indices; Laue method; Bragg method; description of procedure for Debye Scherrer method of X-ray structural analysis of crystals; index reflections.

Identification of unit cells from systematic absences in diffraction pattern-structure of simple lattices and X-ray intensities-structure factor and its relation to intensity and electron density. Powder XRD and Single Crystal XRD working principles.

X-Ray Fluorescence Spectroscopy. Principle, energy dispersive X-ray fluorescence (EDXRF); wavelength dispersive X-ray fluorescence (WDXRF); applications

Unit 4 Nuclear Techniques 15

Basic concepts of nuclear chemistry; radioactive decay and equilibrium; nuclear reactions; Q value; cross sections; types of nuclear reactions; radioactive techniques: counting techniques such as G. M. ionization and proportional counter, isotopic dilution, neutron activation analysis, radiometric titration; radiopharmaceuticals: radioimmunoassay, immunoradiometric assay, classification of radiopharmaceuticals, labeled compounds preparation, PET studies.

Prescribed books:

1. Drago, Russell S. *Physical Methods in Chemistry*. 2nd ed., Saunders College Publishing, 1992.
2. Raj, Gurdeep. *Advanced Physical Chemistry*. 35th ed., Goel Publishing House, 2009.

Reference Books:

1. Glasstone, Samuel. *Electrochemistry*. Methuen & Co. Ltd., 1930.
2. Billmeyer, Fred W., Jr. *Textbook of Polymer Science*. 3rd ed., Wiley-Interscience, 1984.
3. Gowariker, V. R., Viswanathan, N. V., and Sreedhar, Jayadev. *Polymer Science*. Reprint ed., New Age International, 2022.
4. Glasstone, Samuel. *An Introduction to Electrochemistry*. 4th ed., Affiliated East-West Press Pvt. Ltd., 1974.
5. Yadav, M. S. *Electrochemistry*. 2nd rev. ed., Anmol Publications Pvt. Ltd., 2001.
6. Arnikar, H. J. *Essentials of Nuclear Chemistry*. 4th ed., Wiley Eastern, 1995.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Drug Discovery, Design and Development
Category: M.Sc.
Couse Code: 24MCHE3AT
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course aims to provide a strong foundation in pharmacology, drug formulation, and various routes of administration. It covers the principles of pharmacokinetics and pharmacodynamics essential for drug action and delivery. Students will explore lead discovery, optimization strategies, and therapeutic agent design. The course also emphasizes prodrug development and the structure–activity relationships of widely used drugs.

Course Outcomes:
At the end of the course, the student will be able to
1. explain the structure of pharmaceutical industries, drug development stages, and drug formulation types.
2. apply ADME principles and receptor interaction theories to interpret drug behavior in the body.
3. analyze lead discovery and optimization strategies for the rational design of drugs.
4. evaluate the mechanism of action and therapeutic applications of selected drugs using SAR principles.

Unit 1 **Basic Introduction to Pharmaceutical industry and Principles of Pharmacology** **15**

Types of pharmaceutical industries: API, CRO, CRAMS, CDMO; departments: R&D, Process R&D, Analytical R&D, Quality Assurance (QA) / Quality Control (QC); Intellectual Property Rights, Generic and proprietary medicines.
Definitions of disease, drug, bioassay, pharmacokinetics and pharmacodynamics; stages involved in drug discovery; formulation; drug dosing forms: solid dosage forms, semi-solid dosage forms and liquid dosage forms; routes of drug administration

Unit 2 **Principles of Pharmacokinetics, Pharmacodynamics and Drug Delivery** **15**

Absorption, distribution, metabolism and excretion of drugs (ADME); nature of drug - receptor interactions; theories of drug action: occupancy theory, rate theory, Induced-fit theory, drug synergism and antagonism and clinical trials and Concepts of Drug Delivery

Unit 3 **Lead Discovery and optimization** **15**

Lead discovery. Existing drugs as leads (me too drugs); pharmacophore; principles of design of agonists, antagonists and enzyme inhibitors. drug discovery without lead – serendipity-penicillin and librium as examples.
Lead optimization: variation of alkyl substituents; chain homologation and branching; variation of aromatic substituents; extension of structure; ring expansion and ring contraction; ring variation; variation and position of hetero atoms; ring fusion; simplification of the lead; rigidification of lead

Unit 4 Role of AI in diagnosis and Drug discovery applications 15

Introduction to Artificial Intelligence (AI) and Machine Learning (ML) in pharmaceutical sciences. Applications of AI in disease diagnosis, target identification, drug repurposing, and virtual screening. Overview of AI-driven predictive models in ADMET and clinical trials. Case studies on successful AI-enabled drug discovery platforms.

Prescribed books:

1. Singh, Harkishan, and Kapoor, V. K. *Medicinal and Pharmaceutical Chemistry*. 2nd ed., Vallabh Prakashan, 2005.
2. Patrick, Graham L. *An Introduction to Medicinal Chemistry*. 6th ed., Oxford University Press, 2017.

Reference Books:

1. Thomas, Gareth. *Fundamentals of Medicinal Chemistry*. 2nd ed., Wiley, 2016.
2. Nogrady, Thomas, and Weaver, Donald F. *Medicinal Chemistry: A Biochemical Approach*. 3rd ed., Oxford University Press, 2005.
3. Lemke, Thomas L., and Williams, David A., editors. *Foye's Principles of Medicinal Chemistry*. 8th ed., Wolters Kluwer, 2017.
4. Sneha, P. *Artificial Intelligence in Drug Discovery and Development*. CRC Press, 2023.
5. Hassane, A. *Artificial Intelligence in Healthcare and Drug Discovery*. Academic Press, 2021.Kar, Ashutosh. *Medicinal Chemistry*. 4th ed., New Age International, 2013.
6. Nadendla, Rama Rao. *Principles of Organic Medicinal Chemistry*. 2nd ed., New Age International, 2016.
7. Wolff, Manfred E., editor. *Burger's Medicinal Chemistry and Drug Discovery*. 6th ed., Wiley, 2003.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Materials science
Category: M.Sc.
Couse Code: 24MCHE3BT
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course is designed to introduce students to diverse synthesis techniques for nanostructured materials and their characterization using advanced analytical tools. It covers the fundamental principles governing the magnetic and optical properties of materials. The course also explores the mechanisms behind these properties and their practical significance. Special emphasis is placed on material applications in modern energy devices such as fuel cells and batteries.

Course Outcomes:
At the end of the course, the student will be able to
1. explain the principles and processes involved in different synthesis methods for nanomaterials.
2. apply material characterization techniques like XRD, SEM, and TEM to interpret structural and surface properties.
3. analyze magnetic and optical behaviors of materials based on their structure and composition.
4. evaluate the suitability of materials used in fuel cells and batteries based on their physical and electrochemical properties.

Unit 1 Preparation Methods 15
introduction, types of materials. Chemical precipitation and co-precipitation; metal nanocrystals by reduction; sol-gel synthesis; microemulsions or reverse micelles; solvothermal synthesis; microwave heating synthesis; sonochemical synthesis. latest applications of materials in various fields.

Unit 2 Characterization of Materials 15
IR UV X-Ray diffraction (XRD); scanning electron microscopy (SEM); transmission electron microscopy (TEM); BET

Unit 3 Magnetic and Optical Properties of Materials 15
Magnetic properties - dia, para, ferro, anti-ferro and ferri magnetism; measurements - magnetic moment and magnetic susceptibility; optical properties - optical absorption and band gaps; luminescence: principle, characteristics and materials. Applications of optical materials (sensor materials).

Unit 4 Materials for Fuel Cells and Batteries 15
Proton exchange membrane fuel cells; material aspects; lithium battery materials; electrode and electrolyte materials.

Prescribed books:

1. Ozin, Geoffrey A., Arsenault, André C., and Cademartiri, Ludovico. *Nanochemistry: A Chemical Approach to Nanomaterials*. 2nd ed., Royal Society of Chemistry, 2009.
2. Ajayan, Pulickel M., Schadler, Linda S., and Braun, Paul V. *Nanocomposite Science and Technology*. 1st ed., Wiley-VCH, 2003.
3. Wang, Zhong Lin, editor. *Characterization of Nanophase Materials*. 1st ed., Wiley-VCH, 2000.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Multistep Synthesis of Organic Compounds
Category: M.Sc.
Couse Code: 24MCHE34L
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	6	4

Course Objectives: This course aims to provide students with a strong foundation in the theoretical principles and strategic planning of multistep organic synthesis. It emphasizes hands-on training in executing sequential reactions and functional group transformations. Students will gain practical experience in reaction monitoring, product work-up, and purification techniques. The course also focuses on the identification and characterization of synthesized organic compounds using standard methods.

Course Outcomes:
At the end of the course, the student will be able to
1. perform multistep synthesis of complex organic compounds through sequential functional group transformations.
2. execute standard work-up procedures including extraction, drying, and isolation of organic products.
3. apply purification techniques such as recrystallization or chromatography to obtain pure compounds.
4. identify synthesized compounds using physical properties and qualitative analytical methods.

Multistep Synthesis with % yield

a) Synthesis of Benzanilide from Benzophenone
   Benzophenone → Benzophenone oxime → Benzanilide
b) Synthesis of Benzilic acid from benzoin
   Benzoin → Benzil → Benzilic acid
c) Synthesis of p-Bromoaniline from acetanilide
   Acetanilide → p-bromoacetanilide → p-bromoaniline
d) Synthesis of Flavone from o-hydroxyacetophenone
   o-Hydroxyacetophenone →o-benzoyl acetophenone → o-hydroxydibenzoylmethane → flavone
e) Synthesis of Methyl orange from 4-Aminosulphonic acid
   4-Aminosulphonic acid→4-(chlorodiazenyl)benzenesulfonic acid →Methyl orange
f) Synthesis of 2-phenylindole from acetophenone.
   acetophenone → acetophenone phenylhydrazone→ 2-phenylindole
g) Synthesis of symmetrical tribromobenzene from aniline.
   aniline → 2,4,6-tribromoaniline → Symmetrical tribromobenzene
h) Synthesis of anthranilic acid from phthalic anhydride.
   phthalic anhydride → phthalimide→ anthranilic acid

Prescribed books:

1. Li, Jie Jack, Limberakis, Chris, and Pflum, Derek A. *Modern Organic Synthesis in the Laboratory: A Collection of Standard Experimental Procedures*. 1st ed., Oxford University Press, 2008.
2. Mann, Frederick George, and Saunders, Bernard Charles. *Practical Organic Chemistry*. 4th ed., Pearson Education India, 2009.
3. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., and Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*. 5th ed., Pearson, 1996.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Molecular drawing, modeling, synthesis and characterization of selected bioactive molecules
Category: M.Sc.
Couse Code: 24MCHE35L
Semester: III Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	6	4

Course Objectives: This course is designed to build foundational skills in 2D and 3D molecular drawing, along with principles of molecular modeling and docking. It emphasizes the synthesis of bioactive heterocycles using classical and multicomponent strategies. Students gain hands-on experience in purification and spectral characterization using FT-IR and UV-Visible techniques. The course also highlights the relevance of computational tools in drug design and development.

Course Outcomes:
At the end of the course, the student will be able to
1. construct accurate 2D and 3D molecular representations and perform basic molecular modeling and docking studies.
2. synthesize a variety of bioactive heterocycles using classical and multicomponent organic reactions.
3. apply purification methods such as crystallization or extraction in isolating organic compounds.
4. characterize synthesized molecules using FT-IR and UV-visible spectroscopic techniques.

Course content
1. Basics of drawing the 2D structures of organic molecules and their 3D conversions.
2. Molecular docking studies
3. Synthesis, monitoring, purification and spectral (FT-IR and UV-visible) analysis of 7-hydroxy-4-methylcoumarin (hymechromone) by Pechmann condensation.
4. Multi-component Synthesis, monitoring, purification and spectral (FT-IR and UV-visible) analysis of pyrrole derivatives.
5. Multi-component domino synthesis, monitoring, purification and spectral (FT-IR and UV-visible) analysis of 2-aminothiazoles.
6. Synthesis, monitoring, purification and spectral (FT-IR and UV-visible) analysis of methyl (2- acetoxy-2-phenylacetyl) glycinate by Passerini reaction.
7. Synthesis, monitoring, purification and spectral (FT-IR and UV-visible) analysis of dihydropyrimidinones (DHPMs) by Biginelli Reaction.
8. Synthesis, monitoring, purification and spectral (FT-IR and UV-visible) analysis of benzopinacol via photoreduction with % yield (Demonstration only).

Prescribed books:

1. Introduction to ChemDraw Ultra 12: https://staff.emu.edu.tr/sensevpayanilkan/Documents/courses/ITEC107/LECTURE7.pdf
2. Roberts, G. C. K. *Drug Action at the Molecular Level*. University Park Press, 1977.
3. Furniss, B. S., Hannaford, A. J., Smith, P. W. G., and Tatchell, A. R. *Vogel's Textbook of Practical Organic Chemistry*. 5th ed., Longman Scientific & Technical, 1989.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Organic Chemistry – IV
Category: M.Sc.
Couse Code: 24MCHE41T
Semester: IV Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course aims to provide an in-depth understanding of the mechanisms and synthetic applications of oxidation and reduction reactions in organic chemistry. It focuses on the reactivity of non-metallic reagents like boron, phosphorus, sulfur, and silicon compounds. Students will also explore modern strategies of asymmetric synthesis, including substrate, auxiliary, reagent, and catalyst-controlled methods. The course develops students' ability to apply reaction mechanisms and stereochemical principles in designing efficient organic syntheses.

Course Outcomes:
At the end of the course, the student will be able
1. explain the mechanisms and synthetic applications of various oxidation reactions involving organic substrates.
2. apply different reducing agents to achieve targeted reductions in organic synthesis.
3. analyze the bonding and reactivity of non-metallic reagents and predict their roles in organic transformations.
4. evaluate different asymmetric synthesis strategies and apply them in enantioselective organic reactions.

Unit 1 Oxidations **15**

Alcohols to carbonyls. Chromium(VI) oxidants; dimethyl sulfoxide oxidation; periodate oxidation; Oppenauer oxidation; oxidation with manganese dioxide; DDQ; oxidation with silver carbonate.
Alkenes to Epoxides. Peroxide induced epoxidations.
Alkenes to diols. Oxidation with potassium permanganate; osmium tetraoxide; Prévost oxidation and Woodward modification.
Oxidation of alkyl or alkenyl fragments. Selenium dioxide.

Unit 2 Reductions **15**

Nucleophilic Metal Hydrides. $LiAlH_4$; $NaBH_4$; Red-Al; alkoxy aluminates.
Electrophilic Metal Hydrides. BH_3; AlH_3; DIBAL.
Non-metallic Reductions. Diimide reduction; Wolf-Kishner reduction. Dissolving Metal Reductions. Birch reduction; Clemmensen reduction. Heterogeneous Catalytic Hydrogenations.

Unit 3 Non-Metallic Reagents in Organic Synthesis **15**

Electronic structure and bonding in boron, phosphorus and sulphur compounds: reactivity and applications in organic synthesis.
Boron Reagents. Organoboranes in the formation of C–C bonds, alcohols, amines, halogen and carbonyl compounds, free radical reactions of organoboranes: simple boranes and hindered boranes.
Phosphorus Reagents. Formation of C–C double bonds (Wittig and Horner-Wordsworth-Emmons reactions); functional group transformations; eactivity as electrophiles and nucleophiles.

Sulphur Reagents. Sulphurylides: stabilized and non-stabilized, preparation and reactivity, sulphonylcarbanions.
Silicon reagents. Reactions involving β-carbocations and α-carbanions; utility of trimethylsilyl halides; silyl cyanides and triflates

Unit 4 Asymmetric Synthesis 15

Introduction and Terminology. Topicity in molecules: homotopic, heterotopic (enantiotopic and diastereotopic), prochirality nomenclature; Substitution and addition criteria; Pro-R, Pro-S, Re- and Si-faces; stereoselective reactions: enantioselectivity and diastereoselectivity; optical purity: enantiomeric excess and diastereomeric excess.
Strategies in Asymmetric Synthesis.

i) Chiral Substrate Controlled Asymmetric Synthesis. Nucleophilic additions to chiral carbonyl compounds; 1,2-asymmetric induction; Cram's rule; Felkin-Anh model.
ii) Chiral Auxiliary Controlled Asymmetric Synthesis. α-Alkylation of chiral enolates; azaenolates; imines; use of chiral auxiliaries in Diels-Alder reaction and aldol reactions.
iii) Chiral Reagent Controlled Asymmetric Synthesis. Asymmetric reductions using BINAL−H; asymmetric hydroboration using (IPC)2BH and IPCBH2.
iv) Chiral Catalyst Controlled Asymmetric Synthesis. Sharpless and Jacobsen asymmetric epoxidations; asymmetric hydrogenations using chiral Wilkinson bisphosphine and Noyori catalyst; enzyme mediated enantioselective synthesis

Prescribed Textbooks:

1. House, H. O. *Modern Synthetic Reactions*. 2nd ed., W.A. Benjamin, 1972.
2. Carruthers, W., and Coldham, Iain. *Modern Methods of Organic Synthesis*. 4th ed., Cambridge University Press, 2004.

Reference Books:

1. Norman, R. O. C., and Coxon, J. M. *Principles of Organic Synthesis*. 3rd ed., Blackie Academic & Professional, 1993.
2. Carey, Francis A. *Organic Chemistry*. 9th ed., McGraw-Hill Education, 2019.
3. Bruice, Paula Yurkanis. *Organic Chemistry*. 8th ed., Pearson, 2016.
4. Clayden, Jonathan, Greeves, Nick, Warren, Stuart, and Wothers, Peter. *Organic Chemistry*. 2nd ed., Oxford University Press, 2012.
5. Wade, Leroy G., Jr., Simek, Jan William, and Singh, M. S. *Organic Chemistry*. 9th ed., Pearson, 2017.
6. Carey, Francis A., and Sundberg, Richard J. *Advanced Organic Chemistry: Part A: Structure and Mechanisms*. 6th ed., Springer, 2013.
7. Carey, Francis A., and Sundberg, Richard J. *Advanced Organic Chemistry: Part B: Reactions and Synthesis*. 6th ed., Springer, 2013.
8. Powell, P. *Principles of Organometallic Chemistry*. 2nd ed., Springer, 1988.
9. Davis, S. G. *Organo-Transition Metal Chemistry: Applications to Organic Synthesis*. Pergamon Press, 1982.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Organic Spectroscopy
Category: M.Sc.
Couse Code: 24MCHE42T
Semester: IV Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: The main objectives of this course are to provide a comprehensive understanding of the principles, instrumentation, and applications of various spectroscopic techniques used in organic analysis. Students will learn the fundamentals and practical uses of Ultraviolet and Visible Spectroscopy, Infrared Spectroscopy, and both ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) Spectroscopy. The course also covers advanced techniques such as 2D NMR and introduces the principles, instrumentation, methods, and applications of Mass Spectrometry.

Course Outcomes:
At the end of the course, the student will be able
1. interpret UV-Visible and IR spectra to identify functional groups in organic molecules.
2. analyze ^{1}H NMR spectra to determine proton environments and molecular structure.
3. apply ^{13}C and 2D NMR techniques for structural elucidation of organic compounds.
4. interpret mass spectra to determine molecular structure and fragmentation pathways of organic compounds.

Unit 1 UV-Visible and IR Spectroscopy 15

Ultraviolet and Visible Spectroscopy. Various electronic transitions (185-800 nm); effect of solvent on electronic transitions; ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes and conjugated polyenes; Fieser–Woodward rules for conjugated dienes and carbonyl compounds; ultraviolet spectra of aromatic and heterocyclic compounds; steric effect in biphenyls; polycyclic aromatic compounds.

Infrared Spectroscopy. Instrumentation and sample handling; FT-IR. overtones, combination bands and Fermi resonance; factors influencing vibrational frequencies; characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines; detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds).

Unit 2 ^{1}H NMR Spectroscopy 15

Nuclear spin; nuclear resonance; saturation; shielding of magnetic nuclei; deshielding; chemical shifts and its measurements; factors influencing chemical shift; chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines and amides); spin-spin interactions; coupling constant (J): types and classification (ABX, AMX, ABC etc.) of coupling constants; Karplus curve variation of coupling constant with dihedral angle; virtual coupling; chemical exchange; effect of deuteration; hindered rotation; simplification of complex spectra: nuclear magnetic double resonance (spin decoupling); contact shift reagents; nuclear Overhauser effect

Unit 3 ^{13}C NMR Spectroscopy and 2D NMR Techniques 15

^{13}C NMR Spectroscopy. CW and FT techniques; types of ^{13}C NMR spectra: undecoupled, proton- decoupled and off-resonance decoupled (ORD) spectra; ^{13}C chemical shifts; factors affecting the chemical shifts; chemical shifts of organic compounds; calculation of chemical shifts of alkanes, alkenes and alkynes; homonuclear (^{13}C-^{13}C J) and heteronuclear (^{13}C-,^{1}H J) coupling; ^{13}C NMR spectral editing techniques: principle and applications of DEPT.

2D NMR Techniques. Principles of 2D NMR; classification of 2D-experiments; correlation spectroscopy (COSY), HOMO COSY (^{1}H-^{1}H COSY), COSY of *m*-dinitrobenzene, isopentylacetate, hetero COSY (^{1}H,^{13}C COSY); hetero COSY of isopentyl acetate and 4-methyl-2-pentanol; HMQC; HMQC of codeine; long range ^{1}H,^{13}C COSY (HMBC); HMBC of codeine; NOESY; NOESY of 9-benzylanthracene.

Unit 4 Mass Spectrometry 15

Introduction; principle; instrumentation; single and double focusing mass spectrometers; ionization methods: EI, CI, FDI, PDI, LDI, FAB, TSI and ESI; mass analyzers: MSA, ESA, QMA, ITA, TOF, FT and tandem; molecular-ion peak; nitrogen rule; base peak; metastable ion; isotopic abundance; high resolution mass spectrometry (HRMS); index of hydrogen deficiency (IHD); general methods of mass spectral fragmentation; Mc Lafferty rearrangement; ortho effect; factors affecting fragmentation; mass spectral fragmentation patterns of various classes of organic compounds: alkanes, alkenes, alkynes, aromatics, alcohols, alkyl halides, ethers, aldehydes, ketones, carboxylic acids, esters, amines, amides, nitriles, nitro compounds; mass spectral problems with respect to structure determination.

Prescribed Textbooks:

1. Kemp, W. *Organic Spectroscopy*. 3rd ed., Bloomsbury Academic, 2022.
2. Silverstein, R. M., Webster, F. X., and Kiemle, D. J. *Spectrometric Identification of Organic Compounds*. 8th ed., Wiley, 2014.
3. Pavia, Donald L., Lampman, Gary M., Kriz, George S., and Vyvyan, James A. *Introduction to Spectroscopy: A Guide for Students of Organic Chemistry*. 5th ed., Cengage Learning, 2014.

Reference books:

1. Williams, D. H., and Fleming, I. *Spectroscopic Methods in Organic Chemistry*. 7th ed., Springer, 2020.
2. Kalsi, P. S. *Spectroscopy of Organic Compounds*. 9th ed., New Age International, 2023.
3. Lambert, Joseph B., Mazzola, Eugene P., and Ridge, Clark D. *Nuclear Magnetic Resonance Spectroscopy: An Introduction to Principles, Applications and Experimental Methods*. 2nd ed., Wiley, 2019.
4. Macomber, Roger S. *A Complete Introduction to Modern NMR Spectroscopy*. 1st ed., John Wiley & Sons, 1998.

ANNAMACHARYA UNIVERSITY

(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Medicinal chemistry and Natural products
Category: M.Sc.
Couse Code: 24MCHE43T
Semester: IV Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course aims to provide students with a deep understanding of pharmacokinetics, pharmacodynamics, and various drug delivery systems. It will explore drug design methodologies, lead modification strategies, and the structure–activity relationships (SAR) in medicinal chemistry. The course covers the structure, biosynthesis, stereochemistry, and synthesis of naturally occurring terpenoids and steroids. Additionally, students will study the isolation, structural elucidation, physiological action, and synthesis of alkaloids, flavonoids, and isoflavonoids.

Course Outcomes:
At the end of the course, the student will be able
1. explain pharmacokinetic and pharmacodynamic principles along with advanced drug delivery systems.
2. apply concepts of drug design, SAR, and lead modification in the development of pharmaceutical agents.
3. analyze the structure, biosynthesis, and synthesis of important terpenoids and steroids.
4. evaluate the structural elucidation, biological activity, and synthesis of selected alkaloids and flavonoids.

Unit 1 Terpenoids and steroids 15

Terpenoids. General methods of isolation; classification; isoprene rule; structure determination, stereochemistry, biosynthesis and synthesis of camphor, farnesol and zingiberene.
Steroids. Biological importance of steroids; Diel's hydrocarbon and stereochemistry of steroids; structure determination of cholesterol; structure determination and synthesis of androsterone and testosterone; biosynthesis of steroids

Unit 2 Alkaloids, Flavonoids and Isoflavonoids 15

Alkaloids. General isolation methods; classification; general methods of structural elucidation; physiological action; structural elucidation and synthesis of papaverine and reserpine.
Flavonoids and Isoflavonoids. Nomenclature; general methods of structure determination; structure elucidation and synthesis of apigenin, luteolin, quercetin and daidzein.

Unit 3 Basic Principles of Pharmacology and Concepts of Drug Delivery 15

Definitions. Disease, drug, bioassay, pharmacokinetics and pharmacodynamics; stages involved in drug discovery; formulation; drug dosage: solid dosage forms, semi-solid dosage forms and liquid dosage forms; routes of drug administration.
Pharmacokinetics and Pharmacodynamics. Absorption; distribution; metabolism and excretion of drugs (ADME); nature of drug – receptor interactions; theories of drug action: occupancy theory, rate theory, induced-fit theory, drug synergism and antagonism.
Concepts of Drug Delivery. Drug delivery definition; conventional drug delivery; route specific drug delivery; polymer-drug conjugates; PEGylation; diffusion controlled systems; Ficks laws; reservoir systems; non-erodible matrix systems; bio-erodible systems; types of drug delivery systems; clinical trials of drug delivery systems

Unit 4 Drug Design, Lead Modification and SAR 15

Drug Design. Lead discovery; existing drugs as leads (me too drugs); pharmacophore; principles of design of agonists; antagonists and enzyme inhibitors; design of salbutamol, cimetidine and captopril; drug discovery without lead – serendipity-Penicillin and Librium as examples.

Lead Modification Strategies. Bioisosterism; variation of alkyl substituents; chain homologation and branching; variation of aromatic substituents; extension of structure; ring expansion and ring contraction; ring variation; variation and position of hetero atoms; ring fusion; simplification of the lead; rigidification of lead.

Structure-activity Relationship (SAR) Studies. SAR in sulfa drugs, benzodiazepines and taxol analogs; Structure pruning techniques with morphine as example; principles of prodrug design

Prescribed books:

1. Singh, Harkishan, and Kapoor, V. K. *Medicinal and Pharmaceutical Chemistry*. 3rd rev. ed., Vallabh Prakashan, 2012.
2. Patrick, Graham L. *An Introduction to Medicinal Chemistry*. 7th ed., Oxford University Press, 2023.

Reference books:

1. Thomas, Gareth. *Fundamentals of Medicinal Chemistry*. 1st ed., Wiley-Blackwell, 2003.
2. Nogrady, Thomas. *Medicinal Chemistry: A Biochemical Approach*. 3rd ed., Oxford University Press, 2005.
3. Lemke, Thomas L., and Williams, David A., editors. *Foye's Principles of Medicinal Chemistry*. 8th ed., Wolters Kluwer, 2019.
4. Kar, Ashutosh. *Medicinal Chemistry*. 4th ed., New Age International, 2015.
5. Agarwal, O. P. *Natural Products*. 1st ed., Krishna Prakashan Media, 2006.
6. Torssell, K. B. G. *Natural Product Chemistry: A Mechanistic and Biosynthetic Approach to Secondary Metabolism*. 1st ed., John Wiley & Sons, 1983.
7. Kalsi, P. S. *Chemistry of Natural Products*. 1st ed., Kalyani Publishers, 1983.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Industrial Organic Chemistry
Category: M.Sc.
Couse Code: 24MCHE4AT
Semester: IV Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course aims to provide an understanding of the raw materials, chemical processes, and synthesis routes used in industrial organic chemistry, with a focus on petrochemicals. It will explore the structure, classification, synthesis, and applications of various dyes and fluorescent compounds. The course also covers the chemical nature, classification, and industrial processing of oils, fats, waxes, and soap manufacturing. Additionally, students will learn about the types, preparation methods, and industrial significance of natural and synthetic polymers.

Course Outcomes:
At the end of the course, the student will be able
1. explain the industrial preparation and applications of key petrochemicals and their derivatives.
2. describe the classification, synthesis, and industrial use of dyes and fluorescent dye compounds.
3. analyze the properties of oils, fats, and waxes, and explain the principles of soap manufacturing.
4. differentiate between various types of natural and synthetic polymers and evaluate their properties and industrial uses.

Unit 1 Industrial Organic Syntheses – Petrochemicals 15

Introduction; raw material and basic processes; chemical processes used in industrial organic synthesis; petrochemicals; methanol, ethanol, rectified spirit from beer; methylated spirit; proof spirit; preparation of absolute ethanol from rectified spirit; acetaldehyde; acetic acid; isopropanol; ethylene glycol; glycerin; acetone; phenol; ethyl acetate

Unit 2 Dyes 15

Introduction; sensation of colour; colour and constitution; nomenclature; basic operations in dyeing; classification of dyes according to the mode of application; synthesis, reactions and applications of diphenyl methane dyes, triphenylmethane dyes, phthalein dyes, xanthenes dyes, acridine dyes, sulphur dyes, and cyanine dyes. Fluorescent Dyes: synthesis, reactions and applications of Coumarin fluorescent dyes

Unit 3 Oils, Fats, Waxes and Soaps 15

Introduction - distinction between oils and fats; properties and classifications; animal fats and oils; difference between, animal, vegetable and mineral oils; isolation of essential oils and their uses; saponification value; ester value; acid value; iodine value; Wijs method; Reichert meissl value; Henher value; elaiden test; hydrogenation of oils; soap and its manufacture; general consideration in soap making; manufacture of toilet and transparent soaps; oil to be used for soap; cleansing action of soap. Surfactants introduction and types, Micelle formation.

Unit 4 Natural and Synthetic Polymers 15

Introduction; types of polymerization and their utility; Synthesis and applications of phenolic resins, polyurethanes, epoxy resins, alkyd resins, natural and synthetic rubbers, and biodegradable polymers;

thermoplastic and thermosetting polymers; phenolic resins; polyurethanes; epoxy resins; alkyl resins; natural and synthetic rubber; types and their utility; polymer properties and structure

Prescribed Textbooks:

1. Sharma, B. K. *Industrial Chemistry (Including Chemical Engineering)*. 16th ed., Goel Publishing House, 2014.
2. Rao, M. Gopala, and Marshall Sittig. *Dryden's Outlines of Chemical Technology for the 21st Century*. 3rd ed., Affiliated East-West Press, 2010.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Bioinorganic, bioorganic, biophysical chemistry
Category: M.Sc.
Couse Code: 24MCHE4BT
Semester: IV Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
6	-	-	4

Course Objectives: This course aims to provide an understanding of the role of metal ions in biological systems, including their involvement in oxygen transport, electron transfer, and enzyme catalysis. It will explore the mechanisms of metal ion transport, the importance of trace metals, and biological nitrogen fixation. The course will also cover the structure and biological functions of carbohydrates, lipids, and the catalytic behavior of enzymes. Additionally, students will gain insights into the thermodynamic and structural aspects of biomolecules and the physical forces governing biopolymer interactions.

Course Outcomes:
At the end of the course, the student will be able
1. explain the roles of metal complexes in oxygen transport and electron transfer in biological systems.
2. describe the mechanisms of metal ion transport, biological nitrogen fixation, and their therapeutic and physiological relevance.
3. illustrate the structure and function of biomolecules like carbohydrates, lipids, and enzymes in biological processes.
4. analyze the thermodynamics and molecular interactions of biopolymers and their roles in living systems.

Unit 1 Bio-inorganic Chemistry- I 15

Metal complexes as oxygen carriers: Heme proteins – hemoglobin and myoglobin; Non-heme proteins – hemerythrin and hemocyanin; model synthetic complexes of iron, cobalt, and copper. Co-enzymes and metalloproteins: Vitamin B_{12}, carboxypeptidase, superoxide dismutase, catalase, peroxidase.
Electron transfer in biology: Structure and function of metalloproteins involved in electron transfer – cytochromes, iron-sulphur proteins; synthetic models.
Photosynthesis: Role of metal ions and electron flow.

Unit 2 Bio-inorganic Chemistry- II 15

Metal ion transport and storage in biological systems; molecular mechanisms of ion transport across membranes: ionophores and related systems. Calcium in biological systems: calcium in control processes, muscle contraction, secretion, and blood clotting mechanisms. Hydrolytic metalloenzymes: carbonic anhydrase and other enzymes. Biological nitrogen fixation: in-vivo and in-vitro mechanisms. Importance of trace metals: role of metal ions as chelating agents in medicine; trace metal deficiencies and their biological impact; therapeutic uses of metal-based enzymes.

Unit 3 Bioorganic Chemistry 15

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins.

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition- reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

Unit 4 Biophysical Chemistry 15

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of biopolymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane dialosis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Prescribed books:

1. Hughes, Martin N. *The Inorganic Chemistry of Biological Processes*. 3rd ed., John Wiley & Sons, 2021.
2. Rama Rao, A. V. S. S. *Textbook of Biochemistry*. 11th ed., Himalaya Publishing House, 2022.

Reference books:

1. Atkins, Peter, and de Paula, Julio. *Physical Chemistry*. 11th ed., Oxford University Press, 2018.
2. Alberty, Robert A., and Silbey, Robert J. *Physical Chemistry*. 5th ed., Wiley, 2022.
3. Van Holde, Kensal E., Johnson, Curtis, and Ho, Pui Shing. *Principles of Physical Biochemistry*. 3rd ed., Prentice Hall, 1998.
4. Narayanan, P. *Essentials of Biophysics*. 3rd ed., New Age International, 2023.
5. Finar, I. L. *Organic Chemistry, Volume 2: Stereochemistry and the Chemistry of Natural Products*. 6th ed., Pearson Education, 1973.
6. Kalsi, P. S. *Chemistry of Natural Products*. 1st ed., Kalyani Publishers, 1983.
7. Agarwal, O. P. *Natural Products*. 1st ed., Krishna Prakashan Media, 2006.
8. Torssell, K. B. G. *Natural Product Chemistry: A Mechanistic and Biosynthetic Approach to Secondary Metabolism*. 1st ed., John Wiley & Sons, 1983.

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(ESTD UNDER AP PRIVATE UNIVERSITIES (ESTABLISHMENT AND REGULATION) ACT, 2016)
RAJAMPET, Annamayya District, AP – 516126, INDIA

Title of the Course: Spectral Identification of Organic Compounds
Category: M.Sc.
Couse Code: 24MCHE44L
Semester: IV Semester

Lecture Hours	Tutorial Hours	Practice Hours	Credits
-	-	6	4

Course Objectives: This course aims to provide students with a fundamental understanding of UV, IR, ^{1}H-NMR, ^{13}C-NMR, and Mass spectrometry techniques. It focuses on training students to interpret spectral data for the structural elucidation of organic compounds. Students will also develop proficiency in solving composite spectral problems through the correlation and analysis of multi-spectral data. Additionally, the course aims to enhance practical skills in identifying organic reaction intermediates and products using spectral techniques.

Course Outcomes:
At the end of the course, the student will be able to
1. interpret and assign spectral signals to relevant functional groups in organic molecules using UV, IR, NMR, and Mass spectra.
2. elucidate the structure of unknown organic compounds by correlating multi-spectral data.
3. analyze and identify intermediates and products in multi-step reaction sequences using spectral interpretation.
4. demonstrate proficiency in solving composite spectral problems and justifying structure assignments with supporting data.

Composite spectral problems in three modes, 10 examples in each mode:

a) Propose the structures for compounds that fit the given spectral data and assign the spectral values.
b) For the given scheme and spectroscopic data, deduce the structure of compounds I, II and III, and assign the data.
c) Extract data from the given spectra and elucidate the structure from the obtained data with appropriate discussion.

Prescribed books:

1. Kemp, William. *Organic Spectroscopy*. 3rd ed., Bloomsbury Academic (Red Globe Press), 2022.
2. Silverstein, Robert M., Webster, Francis X., and Kiemle, David J. *Spectrometric Identification of Organic Compounds*. 8th ed., Wiley, 2014.
3. Pavia, Donald L., Lampman, Gary M., Kriz, George S., and Vyvyan, James A. *Introduction to Spectroscopy: A Guide for Students of Organic Chemistry*. 5th ed., Cengage Learning, 2014.