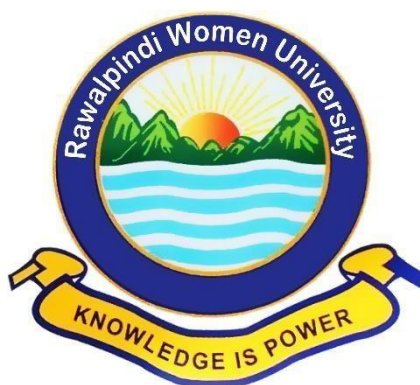


Curriculum Master of Philosophy in Chemistry

(2026)



RAWALPINDI WOMEN UNIVERSITY

Table of Content

A. Departmental Vision

B. Departmental Mission

C. Departmental Objectives

1. Program Objective

2. Admission Requirement

3. Program Design

i. Semester-I

ii. Semester-II

iii. Semester-III/IV

4. Course Codes

5. List of General Courses

6. List of Elective Courses

Table A: Inorganic/analytical chemistry

(Table B): Organic Chemistry

(Table C): Physical Chemistry

(Table D): Applied Chemistry

(Table E): Biochemistry

7. Course Outline of General Courses

8. Course Outline of Inorganic/analytical chemistry

9. Course Outline of Organic chemistry

10. Course Outline of Physical chemistry

11. Course Outline of Applied chemistry

12. Course Outline of Biochemistry

13. List of Elective Courses

A. Department Vision:

To promote women's academic and professional growth in chemical sciences through evolving education, analysis, industrial linkages and sustainable practices, enabling them to contribute meaningfully to scientific advancement and societal betterment.

B. Department Mission:

To empower women through excellence in chemical education and impactful research, fostering leadership and innovation in molecular science, sustainable chemistry, and material design to address global challenges in energy, health, and environment.

C. Departmental Objectives:**1. Academic Excellence**

To provide quality education in basic and advanced chemistry, fostering both theoretical knowledge and psychomotor skills to prepare students for careers in academia, industry, and research.

2. Research and Innovation

To conduct research in various fields of chemistry, encouraging interdisciplinary collaboration and contributions to the advancement of scientific knowledge and technological innovation.

3. Professional Development

To create opportunities for students and faculty to develop professionally, through internships, workshops, seminars, and entrepreneurship that inculcate leadership attributes in them fostering their career in academia, industry, and government.

4. Community Engagement

To collaborate both locally and internationally with industries, government, and community organizations so as to transform lab scale research to real-world solutions.

5. Empowerment of Women

To provide an enabling environment to empower women for their personal and professional development which grooms them to contribute effectively in society.

1. Programme Objective

The main objectives of the program are to:

- Provide a forward-looking curriculum to graduate chemistry students, involving not only traditional chemistry topics but also updated instruction in experimental techniques, computational chemistry and active involvement in professional research.
- Train the graduate students for significant and independent research by offering core chemistry courses, specialization options and advanced computational instruction as well as hands-on involvement in advanced research programs that familiarize students with modern techniques and equipment.

2. Admission Criteria

Admission criteria will be as per university policy.

3. Program Design:

Sr.no	Semester	No. of Courses	Category of Courses	Credit Hours
1.	I	5	1 Core + 3 Elective+ 1 Mandatory	13
2.	II	5	1 Core + 3 Elective+ 1 Mandatory	13
3.	III/IV	1	M.Phil Thesis	06
	Total			32

Semester-I

Sr.no	Course Code	Course Title	Credit Hours	Course Type
1.	CHM-708	Scientific Writing & Research Methods	03	Core
2.		Elective	03	Elective
3.		Elective	03	Elective
4.		Elective	03	Elective
5.	UHQ-101/ ETH-103	Understanding of Holy Quran-I/ Ethics-I	01	Mandatory
			Total=13	

Semester-II

Sr.no	Course Code	Course Title	Credit Hours	Course Type
1.	CHM-709	Advanced Techniques in Chemistry	03	Core
2.		Elective	03	Elective
3.		Elective	03	Elective
4.		Elective	03	Elective
5.	UHQ-102/ ETH-104	Understanding of Holy Quran-II/ Ethics-II	01	Mandatory
			Total=13	

- A list of Courses from TABLE A-F will be offered by the department in category of Elective Courses.

ii. **Semester III and IV**

III and IV semesters are for research and thesis with total 06 credit hours.

4. Course Codes:

- For Inorganic Chemistry course codes are from CHM 710 to CHM-721
- For Organic Chemistry courses codes are from CHM-730 to CHM-739
- For Physical Chemistry course codes are from CHM-750 to CHM-759
- For Applied Chemistry course codes are from CHM-770 to CHM-775
- For Biochemistry course codes are from CHM-790 to CHM-797
- For M.Phil Thesis course code will be CHM-799

The first digit in all course codes represent M.Phil program and next two digits in all codes represent course.

5. List of Elective Courses

Sr.no	Course Code	Course Title	Credit hours
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Table A: Inorganic/Analytical Chemistry

1	CHM-710	Chemistry of Organometallics	3
2	CHM-711	X-Ray Diffraction Techniques	3
3	CHM-712	Advanced Chromatographic Techniques	3
4	CHM-713	Advanced Coordination Chemistry	3
5	CHM-714	Inorganic Electronic Spectroscopy	3
6	CHM-715	Green Chemistry Techniques	3
7	CHM-716	Atmospheric Chemistry	3
8	CHM-717	Metal-Based Drugs	3
9	CHM-718	Thermal Analysis	3
10	CHM-719	Inorganic Material Chemistry	3
11	CHM-720	Purification Process of Metals	3
12	CHM-721	Validation of Analytical Methods	3

Table B: Organic Chemistry

1	CHM-730	Advanced Stereochemistry	3
2	CHM-731	Organic Polymer Chemistry	3
3	CHM-732	Pericyclic Chemistry	3
4	CHM-733	Modern Trends in Asymmetric Synthesis	3
5	CHM-734	Advanced Organic Spectroscopy	3
6	CHM-735	Phytochemical Techniques	3
7	CHM-736	Natural Product Chemistry	3
8	CHM-737	Medicinal Chemistry	3
9	CHM-738	Supramolecular Chemistry	3
10	CHM-739	Advanced Heterocyclic Chemistry	3

Table C: Physical Chemistry

1	CHM-750	Advanced Quantum chemistry	3
2	CHM-751	Applied Nuclear Chemistry	3
3	CHM-752	Advanced Reaction Dynamics	3
4	CHM-753	Polymer and Advanced Composite Materials	3
5	CHM-754	Advanced Statistical Thermodynamics	3
6	CHM-755	Advanced Solid-State Chemistry and Characterization Techniques	3

8	CHM-756	Advanced Photochemistry and Radiation Chemistry	3
9	CHM-757	Surface Chemistry	3
10	CHM-758	Magnetic Spin Dynamics	3
11	CHM-759	Advanced Electrochemistry	3

Table D: Applied Chemistry

1	CHM-770	Advanced Polymer Chemistry	3
3	CHM-771	Physical Structure of Porous Materials	3
4	CHM-772	Agrochemicals	3
5	CHM-773	Industrial Process Chemistry	3
6	CHM-774	Coal Gasification and Liquefaction	3
7	CHM-775	Environmental Impact of Chemical Industries	3

Table E: Biochemistry

1	CHM-790	Enzymes Kinetics	3
2	CHM-791	Drug-Protein and Drug-DNA Interaction	3
3	CHM-792	Bioinformatics	3
4	CHM-793	Clinical Biochemistry	3
5	CHM-794	Biosensors	3
6	CHM-795	Cell Biology	3
7	CHM-796	Industrial Microbiology	3
8	CHM-797	Nutraceuticals Tissue Culture Techniques	3

Table F: List of Additional Elective Courses

Course Code	Table	Credit Hours
CHM-760	Structure Elucidation of Inorganic Materials	3
CHM- 761	Green Chemistry	3
CHM- 762	Nanochemistry and Nanotechnology	3
CHM- 763	Physical Aspect of Polymers	3
CHM- 764	Research Methodology and Statistical Analysis	3
CHM- 765	Advanced Organic Synthesis	3

CHM- 766	Molecular Fluorescence	3
CHM- 767	Named Reactions in Organic Synthesis	3
CHM- 768	Modern Heterocyclic Chemistry	3
CHM- 769	Chirality in Coordination Chemistry	3
CHM- 776	Literature Review and Seminar	3
CHM- 777	Drug Designing and Drug Development	3
CHM- 778	Advanced Analytical Chemistry Techniques	3
CHM- 779	Advanced NMR Spectroscopy	3
CHM- 780	Advanced Atomic Spectroscopy	3
CHM- 781	Sustainable Environmental Chemistry	3
CHM- 782	Solar Cell Chemistry	3
CHM- 783	Advanced Solution and Colloidal Chemistry	3
CHM- 784	Thermodynamic Aspect of Catalysis	3

6. Course Outline of Core Courses

Scientific Writing and Research Methods

Course Code: CHM-708

Credit Hours: 3

Pre-requisite: Nil

Objectives

The students should be able to understand: What is research and why it is carried out, what methodologies need to be adopted, how to write the thesis and research paper, research proposal and get funds.

Learning Outcomes

- Students will be able to learn about fundamentals of writing research synopsis, thesis, and report.
- They will be able to write and submit research proposals and research articles to publish.

Course Outline

Unit 1. Orientation of Course

Research and its classification, research processes.

Unit 2. Research Processes

Tools of data collection, ethics of research, research variables, synopsis.

Unit 3. Research Projects/ Proposal

Thesis write up, article write up, types of research articles

Unit 4. Statistical Analysis in Chemistry

Impact factor, plagiarism, citation, reference format, precision, accuracy, validation, statistical analysis, tools of data collection

Unit 5. Scientific Poster

Use of MS office/excel and end note, chemistry software

Recommended Books/Reference Material

1. C. R. Kothari (2004). "Research methodology; methods and techniques" New Age Publisher.
2. Marczyk, G., DeMatteo, D., Festinger, D., (2005). "Essentials of research design and methodology" John Willey and Sons.
3. Robinson, MS., Stoller, FL., Jones, JK. Robinson, MSC. (2008). "Write like a Chemist" Oxford University Press, NY.
4. Valiela, I. (2008). "Doing Science" Design, analysis and communication of scientific research. Oxford University Press, NY.

Advanced Techniques in Chemistry

Course Code: CHM-709

Credit Hours: 3

Prerequisite: Nil

Objectives:

The objectives of this course is to study the basic analytical techniques and instrumentations.

Course Outcomes:

The students will be able to:

- Basics of electroanalytical techniques
- Working of modern voltametric techniques

Course Outline:

Unit 1. Electroanalytical Techniques

Instrumentation including various kinds of electrodes, modes of operations.

Unit 2. Applications of Electroanalytical Techniques

General applications of electroanalytical techniques in industry, medicine, food and pharmaceuticals.

Unit 3. Electrogravimetry&Coloumetry

Electrogravimetry, controlled–potential coulometry,
constant-current coulometric titrations.

Unit 4. Amperometry Analysis

Amperometric titrations, Dyes and importance, potentiometry.

Unit 5. Modern Voltammetric Techniques

Pulse voltametry, fast linear sweep voltammetry, anodic stripping
voltammetry, cyclic voltammetry.

Recommended books/reference material

1. Brad A.J. Faulkner L.R.; Electrochemical Method: Fundamental and Applications. 2 nd Edition; 2021, John Willey. ISBN; 978-0-471-04372-0.
2. Monk, P.S. Fundamentals of Electroanalytical Chemistry. John-Wiley & Sons Ltd; 2001, ISBN: 0-471-88036-1.
3. Scholz, F. Electroanalytical Methods: Guide to Experiments and Applications. revised Ed.; 2020, Springer-Verlag Berlin, Germany, ISBN: 978-0-471-4372-0.

Course Outline of Elective Courses:

Chemistry of Organometallics

Course Code: CHM-710

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study chemistry of organometallics.

Learning Outcomes

Students should be able to understand:

- Organometallic compounds, their structure, bonding, and reactivity.
- Industrial applications of organometallic compounds.

Course Outline

Unit 1. Synthesis, Bonding and Reactivity

Ionic and metal-carbon sigma bonding in organometallic compounds, factors which make metal-carbon sigma bond in transition metal alkyls kinetically stable and unstable, organolithium compounds, π -metal-ethylene complexes, acetylene complexes, π -Allyl complexes, transition metal complexes with conjugated dienes, metallocenes, π -Arene complexes. Metal carbenes and metal carbynes.

Unit 2.

Organometallic Reactions

Ligand dissociation and substitution, oxidative coupling and reductive extrusions, nucleophilic displacement reactions, insertion and de-insertion reactions, hydride elimination reactions, abstraction.

Unit 3. Organometallic Catalysts

Hydroformylation, hydrogenation by Wilkinson's catalyst, olefin metathesis, Ziegler-Natta polymerizations. Metal-Hydrogen exchange reactions, hydrometallation, oxometalation, water gas reactions.

Recommended books/reference material

1. Gary L. Miessler; Paul J. Fisher and Donald A. Tar. (2014); *Inorganic Chemistry*; (5th Ed.); Prentice Hall.

2. Nathan J. Patmore; Paul I. P. Elliott. (2020), *Organometallic Chemistry*; Volume 43; Royal Society of Chemistry.
3. Perez Pedro; (2021); *Advances in Organometallic Chemistry Research*; (1st Ed.); Volume 76 Academic Press; ISBN: 9780323850698.
4. Powell Peralta. (2013); *Principles of Organometallics Chemistry*; (2nd Ed.), Springer.
5. Robert B. Jordan. (2007); *Reaction Mechanisms of Inorganic and Organometallic Systems*; (3rd Ed.), Oxford University Press, New York; ISBN 978-0-19-530100-7.
6. Robert H. Crabtree. (2019); *The Organometallic Chemistry of the Transition Metals*; (7th Ed); John-Wiley and Sons, New Jersey.

X Ray Diffraction Technique

Course Code: CHM-711

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study X-ray diffraction techniques.

Learning Outcomes

Students should be able to understand:

- The Powder X-ray Diffraction and Single Crystal X-ray Diffraction.
- The determination of molecular and electronic structure of inorganic compounds and metal complexes with the help of different diffraction techniques.

Course Outline

Unit 1. X-Ray Diffraction (XRD)

Structure determination, X-ray crystallography, theory of X-ray diffraction, Bragg's equation, Debye-Scherrer ring, absorption of Xrays, crystals, crystallization, unit cell, asymmetric unit, symmetry operations, Bravais lattices, crystal system/classes, Miller index, phase problem, the direct methods for phase determination, reciprocal lattice.

Unit 2. Powder X-Ray Diffraction

Principles of Powder X-ray diffraction, generation of X-rays, characteristic X-rays, Rietveld method, significance of peak shape in XRD, preparing a powder specimen, powder diffractometer, instrumentation, working of powder X-ray diffraction, spectral contamination in diffraction patterns, Goniometer, identification of compounds, What information obtained from powder X-ray

diffraction?, data collection, results and presentation, application of powder X-ray diffraction, strengths and limitations of X-ray powder diffraction, X-ray diffraction at synchrotron sources.

Unit 3. Single Crystal X-Ray Diffraction

Need for single crystal XRD, comparison between single crystal X-ray analysis and other methods, principles of single-crystal X-ray diffraction, interpretation of data, electron density maps, single crystal structure refinement (SREF), fourcircle or area-detector diffractometer, instrumentation, working of diffractors, data processing, Siemens molecular analytical research tool (SMART), Siemens area detector integration (SAINT), solving a crystal structure by single crystal diffraction techniques, use of SHELXTL and SHELX for the refinement of single crystal data, correct placement of disordered atoms during refinement, applications, strengths and limitations of single-crystal X-ray diffraction, advantages and disadvantages of X-rays, powder diffraction v/s single-crystal X-ray diffraction, neutron diffraction, electron diffraction.

Unit 4. X-Ray Fluorescence Spectroscopy

Theory, history, nature of analytic, types of spectrometer, EDXRF, WDXRF, basic design of XRF spectrometer, EDXRF and WDXRF, source, samples, detectors and analyzers, multi-channel analyzer (MCA), sample holder/cup, primary collimator, analyzing crystals, gas filled detectors, scintillation detectors, duplex detectors, sample preparation for WD-XRF, glass bead sampler, press pellet, advantages and disadvantages of XRF, applications, difference between XRD and XRF, qualitative and quantitative analysis in EDXRF and WDXRF

Recommended books/reference material

1. Cotton. (2007); *Advanced Inorganic Chemistry*; (6th Ed.); Wiley India Pvt. Limited
2. Douglas A. Skoog; F. James Holler; Stanley R. Crouch. (2017); *Principles of Instrumental Analysis*; (7th Ed.); Cengage Learning.
3. James E. Huheey. (2008); *Inorganic Chemistry-Principles, Structure and Reactivity*; Harper and Row Publisher, Inc. New York.
4. John P. Fackler; Larry R. Falvello. (2011); *Techniques in Inorganic Chemistry*; CRC Press.
5. Oliver H. Seeck; Bridget Murphy, (2015), *X-Ray Diffraction: Modern Experimental Techniques*; CRC Press.
6. Peter Atkins; Tina Overton. F. (2010) *Shriver and Atkins Inorganic Chemistry*; (5th Ed.); OUP Oxford.

Advanced Chromatographic Techniques

Course Code: CHM-712

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study advance chromatographic techniques.

Learning Outcomes

Students should be able to understand:

- Understand and apply Gas chromatography, high performance liquid chromatography and super critical fluid chromatography.
- Apply these advanced techniques in designing research ideas and projects.

Course Outline

Unit 1. Common Feature in Advanced Chromatography

Van-dimeter equation, applications of equation, Van-dimeter plots for different chromatographic techniques.

Unit 2. Gas Chromatography (GC)

Theory and instrumentation, advancements in GC including Gas Chromatography-Mass Spectrometry (GC-MS), applications.

Unit 3. High Performance Liquid Chromatography (HPLC)

Theory and instrumentation, advancements in HPLC including High Performance Liquid Chromatography/Mass Spectrometry (HPLC/MS), applications.

Unit 4. Supercritical Fluid Chromatography (SFC)

Amorphous and crystalline structures, Semicrystalline nature, viscoelasticity models and predictions, time-temperature dependency, polymer rheology.

Unit 5. Properties and Applications of Polymers

Supercritical fluids, theory of SFC and instrumentation, applications in organic and pharmaceutical Chemistry. Coupled techniques used especially with chromatography.

Recommended books/reference material

1. Charles G. Smith, (2020), *Handbook of Chromatography*; (1st Ed.); CRC Press; ISBN: 9781351072458.
2. Douglas A. Skoog; Donald M. West; F. James Holler. (2021), *Fundamentals of Analytical Chemistry*. (10th Ed.); Cengage Learning.
3. G.D. Christian. (2013), *Analytical Chemistry*; (7th Ed.); John Wiley & Sons Inc; ISBN: 1118805275.
4. Mark M. Vittha; (2017), *Chromatography: Principles and Instrumentation*; Inc; John Wiley & Sons; ISBN: 9781119270881.
5. R.L. Wixon; C. W. Gehrke. (2022); *Chromatography: A Science of Discovery*; John Wiley & Sons Inc.

Advanced Coordination Chemistry

Course Code: CHM-713

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study advanced coordination chemistry.

Learning Outcomes

Students should be able to understand:

- Thermodynamic and kinetic stability of metal complexes.
- Synthesis and reactivity of complexes under different conditions, and their catalytic applications.

Course Outline

Unit 1. Introduction

Introduction, symmetry elements, symmetry operations, introduction to groups, symmetry points groups, class structure, representations and character tables, chemical applications of group theory.

Unit 2.

Preparation and Reactions of Metal Complexes

Substitution reactions in aqueous solutions, substitution reactions in non-aqueous solvents, substitution reactions in the absence of solvents, thermal dissociation of solid complexes, oxidation-reduction reactions, catalysis, substitution reactions without metalligand bond cleavage, synthesis of cis-trans isomers, isomer enumeration.

Unit 3. Thermodynamic and Kinetic Aspects of Metal Complexes

Stability of metal complexes, kinetically labile and kinetically inert complexes, classification of octahedral complexes into labile and inert complexes on the basis of VBT and CFT, determination of stability of complexes from thermodynamic data, factors affecting the stability of metal complexes, Irving William order of stability, chelation, methods for the determination of stability constants and composition of a complex.

Unit 4. Molecular Rearrangements and Reactions of Coordinated Ligands

Molecular rearrangements in four and six coordinated complexes, reactions due to metal ion polarization of coordinated ligands, hydrolysis of amino acid esters and amides, imine formation, hydrolysis and substituent exchange, macro-cyclic ligands and macrocyclic effect, template effect.

Recommended books/reference material

1. F. A Cotton and G. Wilkinson. (2007), *Advanced Inorganic Chemistry*, (6th Ed.); John-Wiley & Sons, New York.
2. J. E. House. (2019); *Inorganic Chemistry*; Elsevier; ISBN: 0128143703, 9780128143704.
3. James E. Huheey. (2008) *Inorganic Chemistry-Principles, Structure and Reactivity*, Harper and Row Publisher, Inc. New York.
4. Miessler, G.L., Tarr, D. A. (2014); *Inorganic Chemistry*; (5th Ed.), Pearson Education, India; ISBN; 0321811054, 9780321811059.

5. Narayan S. Hosmane. (2017) *Advanced Inorganic Chemistry: Applications in Everyday life*; Elsevier; ISBN; 012801993X, 9780128019931.

Inorganic Electronic Spectroscopy

Course Code: CHM-714

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objectives of this course are to understand the fundamentals of electronic Spectroscopy, explore instrumentation and techniques, study electronic transitions in inorganic complexes, differentiate between high-spin and lowspin complexes, examine charge transfer transitions.

Learning Outcomes

Students should be able to understand:

- Various types of transitions (e.g. d-d transition, charge transfer) occurring in transition metal compounds
- And to characterize new compounds by application of electronic spectroscopy.

Course Outline:

Unit 1. Introduction to Electronic Spectroscopy and Russell-Saunders Coupling Scheme

Overview of electronic spectroscopy, Types of electronic transitions in inorganic compounds, Understanding the electronic configurations and states of transition metal complexes, Application of the Russell-Saunders (LS) coupling scheme to transition metals.

Unit 2. Derivation of Term Symbols for d1-d10 Systems and d-d Transitions

Methods for deriving term symbols for electronic configurations ranging from d1 to d10. Detailed study of d-d electronic transitions within transition metal complexes.

Unit 3. Electronic Structure and Spectroscopic Correlation of Transition Metal Complexes

Connecting Atomic States and Molecular States Linking atomic electronic states to the molecular states of complexes. Correlation diagrams to understand electronic transitions and their selection rules. Tanabe-Sugano Diagrams Interpretation and its construction for predicting electronic transitions. Calculation of 10Dq Values Techniques for calculating the crystal field splitting parameter (10Dq) in various ligand fields.

Unit 4. Advanced Concepts in Transition Metal Complexes

Differentiation between high-spin and low-spin complexes based on ligand field theory. Jahn-Teller Effect Examination of the JahnTeller effect and its implications on the geometry and electronic structure of complexes. Application of subgroup analysis in simplifying complex spectroscopic problems. Selection Rules for Electronic Transitions in Molecules. Exploring the selection rules that govern electronic transitions in inorganic molecules. Ligandto-Metal Charge Transfer (LMCT) and Metal-to-Ligand Charge Transfer (MLCT) and their significance in spectroscopy.

Unit 5. Spectroscopy of Complex Geometries

Case studies and examples illustrating electronic spectroscopy in complexes with various geometries (e.g., octahedral, tetrahedral, square planar)

Recommended Books/reference material:

- C.N.R Rao. Spectroscopy in Inorganic Chemistry; Volume 2; 2012; Elsevier.
- Donald L. Pavia; Gary M. Lampman; George S. Kriz. Introduction to Spectroscopy; 5th Edition; 2015; Cengage Learning.

- Edward I. Solomon; A. B. P. Lever. Inorganic Electronic Structure and Spectroscopy; 2006; John-Wiley & Sons Inc.
- Fabio Bruni; J. Yarwood; Richard Douthwaite. Spectroscopic Properties of Inorganic and Organometallic Compounds; Volume 42; 2011; The Royal Society of Chemistry, UK.
- Mandeep Dalal. A Textbook of Inorganic Chemistry; Volume 1; 2017; Dalal Institute.

Green Chemistry Techniques

Course Code: CHM-715

Credit Hours: 03

Objectives

The objective of this course is to gain a comprehensive understanding of the fundamental principles and goals of green chemistry, including the 12 Principles of Green Chemistry. Learn about sustainable chemical processes and practices that minimize environmental impact, including waste reduction, energy efficiency, and use of renewable resources. Learn about safety considerations and regulatory frameworks related to green chemistry, including guidelines for safe chemical practices and compliance with environmental regulations.

Learning Outcomes

- Students will be able to understand:
 - The concept of green chemistry.
 - Sustainability as course contents as it relates to green chemistry.
 - To understand the basic principles of green chemistry.
 - Differentiate between different types of solvents. How greener solvents are best alternate sources for various synthesis protocols?
 - To develop an understanding of alternate synthesis routes for various industrial products.
 - To develop a skill for energy efficient framework design.

Course Outline

Unit 1. Conducting Polymers and Molecular Weight Determination

Introduction to Green Chemistry: Definition and concept of green chemistry, global movements for sustainable development. (a step towards green chemistry), importance of this new area of chemistry, goals of green chemistry, the roots of innovation and 12 principles of green chemistry.

Unit 2. Tools of Green Chemistry

Alternative feed stocks starting material, alternative reagents, alternative solvents, alternative products /target molecules, process analytical chemistry and alternative catalysts. Focus on the applications of innovative technology, the development of greener” routes to improve industrial processes and to produce important products. Alternative synthetic routes (e.g. C-H bond activation).

Unit 3. Energy Efficiency & Emerging Technologies

Design for energy efficiency photochemical reactions processes, advantages of and challenges faced by photochemical examples of photochemical reactions, chemistry using microwaves, microwave heating, microwaveassisted reactions, sonochemistry and green chemistry examples of electrochemical synthesis

Unit 4. Hydrogen

The clean pollution free fuel, hydrogen fuel from water, fossil fuel, CH₄ and CH₃OH, hydrogen fuel cell technology, mechanism of electricity generation in a fuel cell.

Unit 5. Renewable Resources

Solar Energy, Solar Photovoltaic System (PV cells), solar thermal devices (STD), wind energy, geothermal energy, hydrothermal energy, oceanic power, biomass energy, bio-gas, bio-fuel, biodiesel.

Unit 6. Green Chemistry Using Bio Catalytic Reactions

Introduction, Fermentation and bio transformations, production of bulk and fine chemicals by microbial fermentation, bulk & fine Chemicals, antibiotics, vitamins,

bio catalysis synthesis of industrial chemicals by bacterial constructs, examples of green bio catalytic processes.

Recommended books/reference material

- Bela Torok; Timothy Dransfield. Green Chemistry: An Inclusive Approach; 2017; Elsevier; ISBN: 0128095490, 9780128095492.
- Jimenez-Gonzalez; David, J.C. Green Chemistry and Engineering: A Practical Design Approach, 2011, John Wiley & Sons, ISBN: 978-0-47017087-8.
- Mike Lancaster. Green Chemistry: An Introductory Text. 2nd Edition; 2010, RSC publishing. ISBN: 978-1-84755-873-2.
- R. A. Sheldon; Isabella Arends; Ulf Hanefeld. Green Chemistry and Catalysis. WileyVerlag, 2007, ISBN: 978-3-527-30715-9.
- V.K. Ahluwalia. Green Chemistry: A Textbook; Alpha Science International; 2013 ISBN: 1842657534, 9781842657539
- V.K. Ahluwalia; M. Kidwai. New Trends in Green Chemistry; 2012, Kluwer Academic Publishers. ISBN: 978-94-015-7102-9.

Atmospheric Chemistry

Course Code: CHM-716

Credit Hours: 03

Objectives

The objectives of this course are understand

- The basics of atmospheric chemistry and Identify and understand the sources, effects, and behavior of major atmospheric pollutants, including volatile organic compounds (VOCs), nitrogen oxides (NO_x), sulfur dioxide (SO₂), and particulate matter.
- Furthermore, gain hands-on experience in analyzing atmospheric samples, interpreting data, and applying theoretical concepts to real-world problems.

Learning Outcomes

Students will be able to understand:

- The different regions of the atmosphere and the flow of air within the atmosphere.
- Balance of energy and heat in the atmosphere and how this related to climate.
- Chemistry of ozone in the troposphere through the chemical cycling of Ox, HOx, ROx and NOx.
- Key processes that control the concentration of aerosols in the atmosphere.

Course Outline

Unit 1. Atmosphere and Chemistry

History and evolution of earth atmosphere layers of atmosphere, variation of pressure with height in the atmosphere, composition of atmosphere, energy balance for earth and atmosphere, spatial and temporal scales of atmospheric processes.

Unit 2. Earth's Atmosphere

Major / Minor Gases, sources / sinks of atmospheric gases, airglow, aurora and ions, the life cycle of atmospheric gases, chemical and physical cycles of carbon. Photochemistry of Atmosphere: Introduction to oxygen, ozone, water, nitrogen.

Unit 3. Chemistry of Stratosphere

Calculated troposphere life time of some representative organics. Ozone significance, natural control of ozone, role of CLOx in stratosphere, chlorofluorocarbons in atmosphere probing the ozone shield, ozone hole.

Unit 4. Chemistry of the Atmosphere Aqueous Phase

Properties of Water and Water solutions, specific heat of water and ice, water equilibrium in the atmosphere, cloud and fog formation; isobaric cooling, adiabatic cooling. Other forms of water in atmosphere; Ice clouds, rain and cloud climatology.

Unit 5. Aqueous Aerosols in the Troposphere

Aerosol sources, types of aerosols and aerosol formation mechanisms.

Unit 6. Man's Adverse Influences on the Atmosphere

Photochemical smog, its nature, occurrence, impacts and control measures. The 'Greenhouse Effect', global warming, climate change, and their impacts.

Recommended books/reference material

- Baird, C. and Cann, M., Environmental Chemistry; 5th Edition; 2012; W. H. Freeman & Company.
- Beard, J.M, Murphy, R.A., Environmental Chemistry in Society; 3rd Edition; 2021; CRC Press; ISBN: 9780367313241.
- Trimm, H.H, Hunter, W; Environmental Chemistry: New Techniques and Data; 2021; Apple Academic Press Incorporated; ISBN: 177463192X, 9781774631928.
- Weiner, E.R., Applications of Environmental Aquatic Chemistry; 2021; CRC Press; ISBN: 978-1-4398-5332-0.
- Yaser, A.Z., Khullar, P., Haghi, A.K, Green Materials and Environmental Chemistry; 1st Edition; 2021; Apple Academic Press; ISBN: 9780429330674.

Metal-Based Drugs

Course Code: CHM-717

Credit Hours: 03

Objectives

The objectives of this course are to gain a comprehensive understanding of the principles and historical development of metal-based drugs in medicine. Learn the fundamental principles of designing metal-based drugs, including coordination chemistry, organometallic chemistry, and

bioinorganic chemistry, Understand how metal-based drugs interact with biological macromolecules and their mechanisms of action in various therapeutic contexts and their side effects.

Learning Outcomes

Students should be able to understand:

- The effects of metals in biological systems.
- Action, metabolism, development along with production of different metal-based drugs.

Course Outline

Unit 1. Metals and Neurodegenerative Diseases

Metals in brain, disorders of copper metabolism: wilson's and menkes diseases, aceruloplasminaemia, creutzfeldt-jakob and other prion diseases, iron redox metal ions, oxidative stress and neurodegenerative diseases parkinson's disease, alzheimer's disease, huntington's disease, friedreich's ataxia.

Unit 2.

Drugs and their Action

What are drugs and why do we need new ones? Drug discovery and design, sources of drugs and lead compounds, drug synthesis, market forces and 'me-too drugs, routes of administration, the pharmaceutical phase, drug action, the pharmacokinetic phase, absorption, distribution, metabolism, elimination, bioavailability of a drug, the pharmacodynamic phase.

Unit 3.

Drug Metabolism

The stereochemistry of drug metabolism, biological factors affecting metabolism, environmental factors affecting metabolism, species and metabolism, secondary pharmacological implications of metabolism, sites of action, phase I metabolic reactions, phase II metabolic routes, pharmacokinetics of metabolites, drug metabolism and drug design. Drug development and production: Chemical development, chemical engineering issues, chemical plant, health and safety considerations, synthesis quality control, pharmacological and toxicological testing, drug metabolism and pharmacokinetics, formulation development, production and quality control, patent protection, regulation.

Unit 4. Metals in Medicine

Metallotherapeutics with lithium, cisplatin: an anti-cancer drug, contrast agents for magnetic resonance imaging, metals in the environment, cadmium, aluminum.

Unit 5. Toxicity and Safety of Metal-Based Drugs

Understanding metal toxicity and its impact on health, Monitoring and managing side effects, Guidelines and regulations for metalbased drug approval.

Recommended Books/reference material

1. Crichton, R.R. Biological Inorganic Chemistry, A new introduction to molecular structure and function, 3rd Edition; 2018.
2. Crichton, R.R., Ward, R.J. Metal Based Neuro-degeneration: From Molecular Mechanisms to Therapeutic Strategies, John Wiley and Sons, Chichester, 2006.

Dabrowiak May 2, 2017.
3. Metals in Medicine (Inorganic Chemistry: A Textbook Series) by James C.

4. Thomas, G. Fundamentals of Medicinal Chemistry, John Wiley and Sons, Inc., 605 Third Avenue, New York, NY 10158–0012, USA.
5. Voet, D., Voet, J.G. Biochemistry, 5th Edition; 2016, Wiley, Hoboken, NJ.

Thermal Analysis

Course Code: CHM-718

Credit Hours: 3

Pre-requisite: Nil

Objectives

The objective of this course are, to understand different thermal techniques, their points of similarities and differences. Apply these concepts of thermal techniques in research designing.

Learning Outcomes

- Students will have understanding of different thermo-analytical techniques, their instrumentation and measurement properties.
- They will have command on thermal analysis, instrumentation and various applications of thermal analysis.

Course Outline:

Unit 1. Thermogravimetry (TG)

Principle, instrumentation, balance, furnace, atmosphere control, crucible, thermocouple, temperature control, data collection, applications.

Unit 2. Differential Thermal Analysis (DTA)

Differential Scanning Calorimetry (DSC): Principle, comparison of principles of DTA and DSC, instrumentation, sampling, quantitative aspects of DTA and DSC curves, automation, determination of phase diagram, applications
Thermometric Titrations (TT): Instrumentation, principle, sampling, calibration, applications. Dynamic and Thermo Mechanical analysis (DMA)/ (TMA): Instrumentation, principle, sampling, calibration, applications

Unit 3. General Considerations

Common features and traceability of thermal analysis methods, heating and cooling curve analysis, sources of errors, characterization of the measured curves, and interpretation of data.

Recommended Books/reference material

1. El-Zeiny Ebeid, Mohamed Zakaria., (2021), *thermal analysis from introductory fundamentals to advanced applications*, 1st Edition, Book ISBN: 9780323901925.
2. Haghi, A. K. Thomas, Sabu Palit, Sukanchan Main, Priyanka. (2021), *Methodologies and Applications for Analytical and Physical Chemistry*, Editon 1st.
3. Kenkel, John, (2019), *Analytical Chemistry Refresher Manual*, Edton 1st.
4. Speyer, R.F., (1994), *thermal analysis of materials*, Marcel Dekker Inc. New York., ISBN: 0- 8247-8963-6 780824 789633.
5. Thermal Analysis, (2021), from *introductory fundamentals to advanced applications*.

Advanced Inorganic Material Chemistry

Course Code: CHM-719

Credit Hours: 3

Pre-requisite: Nil

Objectives

The objective of this course are as follow

Students should be able to understand

- Various types of inorganic materials and their crystal structure. The Synthesis, characterization and applications of materials in various fields.

Learning Outcomes

- Students will have understanding of different types of inorganic materials and their crystal structure.
- They will have command on the synthesis, characterization and various applications about materials.

Course Outline:

Unit 1. Inorganic Materials

The technology of materials, types of materials, structure and bonding, relations to other disciplines, crystal chemistry, amorphous solids and icosahedral phases. Boron and borides, carbides and nitrides, oxides, intermetallics, intrinsic properties of inorganic materials, defect chemistry.

Unit 2.

Synthesis and Design of Inorganic Materials

Synthesis from liquids, Gas-phase techniques, Requirements and constraints of material design, Combination properties of composites and their fabrication, Functional materials.

Unit 3. Inorganic Morphogenesis

The chemistry of microstructure and nanostructure, extrinsic properties of materials, fractal dimensions, the chemistry of fractal distribution.

Recommended Books/reference material

1. Housecraft, C. and Sharpe, A. G., (2012), *Inorganic Chemistry*, 4th Edition; Prentice Hall.
2. Narayan S., _____ Hosmane, (2017), *Advanced Inorganic Chemistry: Applications in Everyday Life*, 276 pages.
3. Rodgers G. E. (2012), *Descriptive Inorganic, Coordination, and SolidState Chemistry*, 3rd Edition, Brooks- Cole.
4. Ulrich Schubert, Nicola Hüsing, (2012), *Synthesis of Inorganic Materials*, John Wiley & Sons, 3rd edition.
5. Xu, R., Pang, W., Huo, Q., (2011), *Modern Inorganic Synthetic Chemistry*, 1st Edition; Elsevier.

Purification Process of Metals

Course Code: CHM-720

Credit Hours: 3 Pre-requisite: Nil

Objectives:

Students should be able to understand the Present status of purification of metals.

- Advance methods for purifications of metals.

Learning Outcomes

- Students will have understanding of different purification techniques about metals.
- They will have command on advanced purification techniques of metals.

Course Outline:

Unit 1. Fundamentals for Purification of Metals

Present status of purification of metals, Principles of metal purification and purity evaluation.

Unit 2. Purification Techniques

Pyrometallurgical refining, Hydrometallurgical purification, electrochemical purification, Solid-liquid equilibrium, Selective volatilization, Electrotransport.

Unit 3. Advance Methods for Purifications of Metals

Hydrogen plasma arc melting, Ion-beam deposition, Isotope separation by LASER techniques.

Unit 4. Purification of Selected Metals

Transition metals, Refractory metals, Rare earth metals.

Recommended Books/reference materials

1. Abel Engh, Geoffrey K. Sigworth, et al. (2021), *Principles of Metal Refining and Recycling* by Thorvald Oct 23.
2. Jack Zhang; Baodong Zhao; Bryan Schreiner. (2016), *Separation Hydrometallurgy of Rare Earth Elements*, 1st Edition, Springer; ISBN-13: 978-3319282336.

3. Muhammad Shamsuddin. (2016), *Physical Chemistry of Metallurgical Processes*; 1st Edition; Wiley-TMS; ISBN-13: 978-1119078333.
4. Tao Jiang; Jiann-Yang Hwang; Mark E. Schlesinger; Onuralp Yucel; Rafael Padilla; Phillip J. Mackey; Guifeng Zhou. (2014), *5th International Symposium on High Temperature Metallurgical Processing*, 1st Edition; Wiley-TMS; ISBN-13: 978-1118888117.
5. Yoshio Waseda, Minoru Isshiki. (2012), *Purification Process and Characterization of UltraHigh Purity Metals: Application of Basic Science to Metallurgical Processing*; Springer, ISBN-13: 978-3642625305.

Validation of Analytical Methods

Course Code: CHM-721

Credit Hours: 3

Pre-requisite: Nil

Objectives:

The main objective of this course are the;

- Understanding fundamental concepts on validation and statistical parameters relating validation. To develop standard method of analysis in well planned research.

Learning Outcomes

- Students will gain an understanding about different validation and statistical parameters related to validation.
- They will have command on developing standard method of analysis in a research **Course Outline:**

Unit 1. Requirements

Validation, Method transfer, Statistical parameters and analytical figures of merit.

Unit 2. Method Selection

Terms, Sampling, Fitness for purpose, sources and strategies, sampling considerations.

Unit 3.

Method Development

Mapping the analytical process, determining important factors, Experimental design, Development and validation of analytical design.

Unit 4.

Method Validation

Steps towards method validation, description of the process, data evaluation and reporting, bio-analytical method validation.

Recommended books/reference materials

1. Haghi, A. K, Thomas, Sabu, Palit, Sukanchan, Main, Priyanka. (2020), *Methodologies and Applications for Analytical and Physical Chemistry*, Edition 1st.
2. Kenkel, John. (2019), *Analytical Chemistry Refresher Manual*, Edition 1st.
3. Mark Thomas Stauffer. (2018), *Calibration and Validation of Analytical Methods-A Sampling of Current Approaches*.
4. Tibor Bujdosa, Erna 'Schubert, Andrais. (2020), *Literature of Analytical Chemistry*, Braun, Edition 1st.
5. Trimm, Harold H. (2021), *Analytical Chemistry*, Edition 1st.

Advanced Stereochemistry

Course Code: CHM-730

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study Stereochemical features of organic molecules, Methods used for asymmetry induction in organic compounds and Asymmetric reactions and their use in the synthesis of natural products

Learning Outcomes

- Students will have understanding of Stereochemical features of organic molecules.

- They will have command on asymmetric induction and asymmetric reactions.

Course Outline

Unit 1. Introduction to Chirality

Understanding the concept of chirality in molecules and historical context and significance in science.

Unit 2. Discussion of Chirality

Chirality of chiral carbons, allenes, biphenyls, stereochemical terminology for sugars, amino acids.

Unit 3. Stereochemistry

Identifying stereochemical relationships, pseudoasymmetric compounds, molecules with two chiral centers, prostereoisomerism, prochirality, enantiotopic, diastereotopic groups.

Unit 4. Chiroptical Properties

Chirality in molecules devoid of chiral centers, stereochemistry of alkenes, conformation of acyclic molecules, configuration and conformation of cyclic molecules.

Unit 5. General Concepts in Asymmetric Synthesis

General strategies for asymmetric/Stereoselective synthesis, asymmetric reactions of alkenes, asymmetric additions to aldehydes and ketones, asymmetric reactions in the synthesis of natural products.

Recommended books/reference material

1. Welch, C. J. (2020). William H. Pirkle: Stereochemistry pioneer. *Chirality*, 32(7), 961-974.
2. Wang, P. Z., Xiao, W. J., & Chen, J. R. (2023). Light-empowered contra-thermodynamic stereochemical editing. *Nature Reviews Chemistry*, 7(1), 35-50.
3. Lodochnikova, O. A., Gerasimova, D. P., & Plemenkov, V. V. (2021). From classical to supramolecular dynamic stereochemistry: Double

crystallization-induced diastereomerization of thiazine sulfonamide.
Chirality, 33(7), 409-420.

4. Ahluwalia, V. K. (2022). *Stereochemistry of organic compounds*. Springer.
5. Koskinen, A. M. (2022). *Asymmetric synthesis of natural products*. John Wiley & Sons.

Organic Polymer Chemistry

Course Code: CHM-731

Credit Hours: 03

Pre-requisite: Nil

Objectives

After studying this course, students should be able to understand

- Natural and synthetic polymers, their mechanism and kinetics.
- Structure property relationship and stereochemistry of polymers and Industrial applications of polymers.

Learning Outcomes

- Students will have understanding of natural and synthetic polymers.
- They will have command on mechanisms, kinetics and applications of polymers

Course Outline

Unit 1. Natural and Synthetic Polymers

Classification of polymers, mechanism and kinetics step growth.

Unit 2. Types of Polymerization

Free radical addition and ionic polymerization, ziegler-natta polymerization,

Unit 3. Stereochemistry and Stereo-regulation

Stereochemistry and stereo-regulation of isotactic, atactic and syndiotactic polymers molecular, absolute and relative molecular weight of polymers.

Unit 4. Structure Property Relationship

Reaction of synthetic polymers, polymers degradation and stability, special emphasis on thermal and photo-degradation.

Industrial applications of polymers.

Unit 5. Applications

Applications of natural organic polymers.

Recommended books/reference material

1. Koltzenburg, S., Maskos, M., & Nuyken, O. (2023). *Polymer chemistry*. Springer Nature.
2. Mohamed, M. G., EL-Mahdy, A. F., Kotp, M. G., & Kuo, S. W. (2022). Advances in porous organic polymers: Syntheses, structures, and diverse applications. *Materials Advances*, 3(2), 707733.
3. Parida, S. K., Satpathy, A., Dalai, A., & Mishra, S. (2024). Introduction of Polymers and Polymer Composites: Basic Fundamentals. In *Polymer Composites: Fundamentals and Applications* (pp. 1-37). Singapore: Springer Nature Singapore.
4. Christie, R., & Abel, A. (2021). Organic pigments: general principles. *Physical Sciences Reviews*, 6(12), 807-834.

Pericyclic Chemistry

Course Code: CHM-732

Credit Hours: 03

Pre-requisite: Nil

Objectives

After studying this course, students should be able to understand

- Woodward-Hoffman rule and its application for prediction of reaction products.
- They will have command on pericyclic reactions to other rearrangements and processes and reaction mechanisms and requirements for reaction reagents and conditions.

Learning Outcomes

- Students will have understanding of pericyclic reactions and reaction mechanisms

- They will command on Woodward-Hoffman rule and its application for prediction of reaction products.

Course Outline

Unit 1. Introduction to Pericyclic Reactions

Overview of pericyclic reactions. Characteristics of concerted processes and cyclic transition states

Unit 2. Pericyclic Reactions

Molecular orbitals and their symmetry, molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system, and their symmetry properties

Unit 3. Characteristics and Classification of Pericyclic Reactions

Electrocyclic reactions, conrotatory and disrotatory motions, $4n$, $4n+2$ and allyl systems, woodward-hoffmann correlation diagrams, fmo and pmo approach cycloadditions.

Unit 4. Antarafacial and Suprafacial Additions

Antarafacial and suprafacial additions. $4n$ and $4n+2$ systems, $2+2$ addition of ketenes, ene synthesis.

Unit 5. Sigmatropic Rearrangements

Suprafacial and antarafacial 1,3- and 1,5- shifts of h, sigmatropic shifts involving carbon moieties, 2,3-, and 3,3-sigmatropic rearrangements. claisen, cope, aza-cope, sommlet-hauser, and fischer indole rearrangements.

Recommended books/reference material

1. Vogel, P., & Houk, K. N. (2022). Organic chemistry and synthesis rely more and more upon catalysts. *Catalysts*, 12(7), 758.
2. Izak-Nau, E., Campagna, D., Baumann, C., & Göstl, R. (2020). Polymer mechanochemistry-enabled pericyclic reactions. *Polymer Chemistry*, 11(13), 2274-2299.
3. Mita, T., Takano, H., Hayashi, H., Kanna, W., Harabuchi, Y., Houk, K. N., & Maeda, S. (2022). Prediction of high-yielding

single-step or cascade pericyclic reactions for the synthesis of complex synthetic targets. *Journal of the American Chemical Society*, 144(50), 22985-23000.

4. Fleming, I. (2015). *Pericyclic reactions*. Oxford University Press, USA.

Modern Trends in Asymmetric Synthesis

Course Code: CHM-733

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand and develop the approach for synthetic strategies. They will be able to design total synthesis of organic molecules.

Learning Outcomes

- Students will have understanding of approaches for synthetic strategies.
- They will command on designing total synthesis of organic molecules.

Course Outline

Unit 1. Synthetic Design

Retrosynthetic analysis, reversal of carbonyl group polarity (umpolung), steps in planning a synthesis, choice of synthetic method, domino reactions.

Unit 2. The Concept of Protecting Functional Groups

Protection of NH groups, protection of OH groups of alcohols, protection of diols as acetals, protection of carbonyl groups in aldehydes and ketones, protection of the carboxyl group, protection of double bonds, protection of triple bonds. making carbon-carbon bonds: the orthostrategy for aromatic compounds σ complexes of metals, controlling the michael reaction, specific enol equivalents, extended enolates, allyl anions homoenolates, acyl anion equivalents, synthesis of double bonds of defined stereochemistry, stereo-controlled vinyl anion equivalents.

Unit 3. Electrophilic Attack on Alkenes Vinyl Cations

Palladium-catalyzed c–c coupling allyl alcohols, allylcation equivalents.

Unit 4. Stereochemistry

Control of stereochemistry-controlling relative stereochemistry, resolution, the chiral pool-asymmetric synthesis with natural products as starting materials, asymmetric induction and reagentbased strategy, asymmetric induction, asymmetric catalysis: formation of C-O and C-N bonds, formation of C-H and C-C bonds, asymmetric induction

Unit 5. Substrate Based Strategy

Substrate based strategy, strategy of asymmetric synthesis, classics in total synthesis: vinblastin, plicamine, okaramine, vit b12, rapamycin, taxol, brevetoxin b.

Recommended books/reference material

- 1.Wang, Q., Qi, Y., Gao, X., Gong, L., Wan, R., Lei, W., ..& Walsh, P. J. (2023). Recent trends and developments in the asymmetric synthesis of profens. Green Synthesis and Catalysis, 4(2), 89-103.
- 2.Zweifel, G. S., Nantz, M. H., & Somfai, P. (2017). Modern organic synthesis: an introduction. John Wiley & Sons.
- 3.Seeman, J. I. (2018). On the relationship between classical structure determination and retrosynthetic analysis/total synthesis. Israel Journal of Chemistry, 58(1-2), 28-44.#
- 4.Novaes, L. F., Liu, J., Shen, Y., Lu, L., Meinhardt, J. M., & Lin, S. (2021). Electrocatalysis as an enabling technology for organic synthesis. Chemical Society Reviews, 50(14), 7941-8002.
- 5.Winkler, C. K., Schrittwieser, J. H., & Kroutil, W. (2021). Power of biocatalysis for organic synthesis. ACS central science, 7(1), 55-71.

Advanced Organic Spectroscopy

Course Code: CHM-734

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to

- study advanced spectroscopic studies and organic compounds structural elucidation **Learning Outcomes**
- Understand the concept of advanced and instrumental aspects of different spectroscopic techniques.
- Apply the knowledge in structural elucidation of organic compounds using spectral data.

Course Outline

Unit 1. Ultraviolet/Visible Spectroscopy

Absorption of radiations and electronic transitions, intensities of absorptions, effect of solvents on absorptions, instrumentation, sample handling, chromophore, absorption by conjugated systems, absorption by aromatic compounds, and applications of ultraviolet/visible spectroscopy.

Unit 2. Infrared Spectroscopy

Vibrational modes and absorption frequencies, factors influencing absorption frequencies, intensities, instrumentation, sample handling, interpretation of infrared spectra, characteristic absorption frequencies of some common functional groups, FT-IR, applications of infrared spectroscopy.

Unit 3. ¹H-NMR and ¹³C-NMR

Chemical shift, factors affecting chemical shift, spin relaxation, spin-spin coupling, coupling constants, nuclear overhauser effect, 2-d nuclear magnetic resonance (nmr), correlation spectroscopy (cosy), total correlation spectroscopy (tocsy), nuclear overhauser effect spectroscopy (noesy), rotating frame nuclear overhauser effect spectroscopy (roesy), heteronuclear single-quantum correlation (hsqc) spectroscopy, heteronuclear

multiple quantum correlation (hmqc), heteronuclear multiple-bond correlation (hmbc) spectroscopy.

Unit 4. Mass Spectrometry

An introduction to mass spectrometry, mass spectrometers, ionization techniques, different fragmentation patterns and structure elucidation of compounds.

Unit 5. Combined Application of Organic Spectroscopic Techniques

Combined usage of IR, UV, NMR and mass spectrometric data for structure elucidation of organic compounds having medium and high complexity. electron impact (ei) spectra, chemical ionization (ci) spectra, field desorption (fd) spectra, fast atomic bombardment (fab) spectra, electron spray ionization (esi) spectra, gas chromatography-mass spectrometry, liquid chromatography-mass spectrometry.

Recommended books/reference material

1. Gerson, F., Huber, W. Electron Spin Resonance Spectroscopy of Organic Radicals. 2nd Edition; 2003, Wiley-VCH Verlag GmbH & Co. KGaA. Weinheim, ISBN: 978- 661052033-6.
2. Gunther, H. Basic Principles, Concept, and Applications in Chemistry. 2nd Edition; 2001, John Wiley & Sons, Chichester: New York, USA, ISBN: 0-471-95199-4.
3. Mohan, J. Organic Spectroscopy: Principle and Applications. 2nd Edition; 2009, Narosa Publishing House Pvt. Ltd., ISBN: 978-817319-566-2.
4. Pavia, D.L., Kriz, G.A. Introduction to Spectroscopy. 4th Edition; 2009, Harcourt Brace College Publishers, ISBN: 978-0-49511478-9.
5. Silverstein, R.M., Webster, F.X. Spectrometric Identification of Organic Compounds. 8th Edition; 2015, Wiley: New York, ISBN:

10: 0471393622.

6. Williams, D.H., Fleming, I. Spectroscopic Methods in Organic Chemistry. 5th Edition; 2004, McGraw-Hill companies: New York, ISBN: 0-07-709147-7.

Phytochemical Techniques

Course Code: CHM-735

Credit Hours: 03

Pre-requisite: Nil

Objectives

• The objective of this course is to study about herbs production, their extraction and purification processes **Learning Outcomes**

- The concepts of botanical production of herbs.
- Method of extraction, separation & purification of phytochemicals.

Course Outline:

Unit 1. Herbal Production Processes

Cultivation, collection, cleaning, drying, packaging, and selection of plant parts for phytochemical analysis.

Unit 2. Methods of Extraction

Solvent extraction, maceration, percolation, cold percolation, distillation

Unit 3. Soxhlet Extraction Methods of Extraction

Steam distillation, soxhlet extraction, purification and concentration of miscella, qualitative phytochemical screening.

Unit 4. Methods for Separation of Phytochemicals

Thin layer chromatography, paper chromatography detection and identification of compounds, qualitative and quantitative estimation of phytochemicals.

Unit 5. Bioassay-Study Design

Anti-microbial Studies, anti-inflammatory studies, anti-cancer studies, anti-hyperuricemic studies and toxicity studies of phytochemicals, Introduction to In silico studies.

Recommended books/reference material

1. Mohan, V. R., Tresina, P. S., Doss, A. The Phytochemical and Pharmacological Aspects of Ethnomedicinal Plants, 2021. ISBN: 9781771889544
2. Ramman N., Phytochemical Techniques, New India Publishing Agency, pitamapura, New Delhi, 2015.
3. Raaman, N. Phytochemical Techniques. New India Publishing Agency, Pitam Pura, New Dehli, 2006. ISBN: 81-89422-30-8.

Natural Product Chemistry

Course Code: CHM-736

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study about natural products, their formulation and evaluation.

Learning Outcomes

- The concepts of natural products, their isolation and structure elucidation as well the chemistry and biosynthesis of phytochemicals.
- Formulation and evaluation of Ayurvedic and Herbal medicinal dosage form.

Course Outline

Unit 1. Natural Products

Natural products phytochemicals, enzymatic & biological activity, phytochemical screening, activity directing and structure elucidation directing isolation, chemo taxonomical studies.

Unit 2. Purification of Natural products

Purification methods of natural products, qualitative & quantitative analysis of natural products.

Unit 3. Chemistry of Lignans, Saponins and Tannins

Origin, complex structures, synthesis and biosynthesis (arc1, arc2, arc3), oxidative and epoxide cyclization of squalene.

Unit 4.

Ayurvedic and Herbal Medicine

Extraction and preliminary phytochemical screening, preparation of herbal dosage form, in-vitro & in-vivo study (hepatoprotective, antidiabetic, antioxidant, antitumor), formulation of herbal tablet, pre and post formulation studies, pharmacological investigation (oral acute toxicity studies), drug excipient compatibility.

Unit 5. Terpenoids

Skeletal modification in β -amyrine, lupane and hopane series in terpenoids, classification, nomenclature and isolation technique, properties, extraction and general methods of structure determination of terpenoids, pharmaceutical application

Recommended books/reference material

1. Cane D.F., Barton D.H.R., Nakanishi K. and Meth-Cohn O., Comprehensive Natural Products Chemistry, Elsevier Science Ltd. Vol. 2, 2001.
2. Leeper F.J., Biosynthesis, aromatic polyketides, Springer Verlag, 2000.

Medicinal Chemistry

Course Code: CHM-737

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study about basic principles of medicinal chemistry and drug development

Learning Outcomes

- Review the basic principles that govern medicinal chemistry

- Explore the structure-activity principles in a variety of chemical structures
- Demonstrate fundamental critical thinking skills, including pattern recognition and analogous reasoning
- Critically discuss the rational development of a new drug or therapy.

Course Outline

Unit 1. Introduction to Medicinal Chemistry and History

Drug discovery, drug-target interactions, pharmaceutical properties, drug development process, drug targets

Unit 2.

Drug Design and Modeling

Drug design and development, computer modeling and rational drug design, structure-activity relationships, pharmacokinetics, and pharmacodynamics, known receptor sites, 3D structure of macromolecular targets, structure-based drug-design, ligand-based drug design.

Unit 3.

Drug Metabolism

Drug metabolism principles- Phase I and Phase II. Factors affecting drug metabolism including stereo chemical aspects

Unit 4.

Physicochemical Properties of Organic Medicinal Agents

Solubility, partition coefficient, dissociation constant, hydrogen bonding, chelation, molar refractivity, Ionisation, surface activity, protein binding, bioisosterism, optical and geometrical

Unit 5.

Histamine & Antihistamine

Histamine and antihistamine receptors, H1 antagonists, H2 antagonists

Recommended books/reference material

1. Ashutoshkar, Medicinal Chemistry, New age international (p) limited, publishers, New Delhi, 2007.
2. Donald C. Essentials of Pharmaceutical Chemistry, 4 th Edition, 2012.

3. Eric F., Wolfgang L. Chirality in Drug Research, 1st Edition, 2006.
4. Ganellin C.R., Fischer J. Analogue-Based Drug Discovery, 1st Edition; 2006, ISBN: 3-527-31257-9.
5. Georg T.V., Thomas G., Fundamentals of Medicinal Chemistry, 1st Edition; 2003.
6. John. C., Advance Pharmaceutics, CRC Press, 2004.
7. Thomas G., Fundamentals of Medicinal Chemistry, John Wiley, 2020.

Supramolecular Chemistry

Course Code: CHM-738

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Understand the fundamental principles of supramolecular chemistry and molecular recognition.
- Develop the ability to design and analyze supramolecular systems and devices.

Learning Outcomes

- Analyze various supramolecular interactions and their roles in molecular recognition.
- Design and evaluate synthetic supramolecular systems and their applications in catalysis and molecular devices.

Course Outline

Unit 1. Fundamentals of Supramolecular Chemistry

Supramolecular interactions: ion-ion interactions, ion-dipole interactions, dipole-dipole interactions, hydrogen bonding, cation π interactions, π - π interactions, van der Waals interactions, hydrophobic effect, metal coordination bonds.

Unit 2. Host-Guest Chemistry

Hosts for cation binding, Hosts for anion binding, Hosts for the binding of neutral guests, Synthetic considerations, Templatation,

Kinetic and thermodynamic aspects of binding selectivity,
Templates and supramolecular assemblies, Programmed
supramolecular systems.

Unit 3. Kinetics and Thermodynamics in Supramolecular Systems

Kinetic and thermodynamic considerations, Self-assembled
closed shell compounds, Helicates

Unit 4.

Supramolecular Chirality and Catalysis

Supramolecular chirality: chirality in self-assembled systems,
chirality of host guest compounds, chirality of interlocked
systems, Kinetic models, Supramolecular catalysts, Inner phase
chemistry, Enzyme models.

Unit 5. Self-Replicating Systems and Molecular Devices

Kinetic models of self-replicating systems, Self-replication in
nature, Artificial self-replicating systems, Molecular and
supramolecular devices, Molecular electronic devices,
Switches, Molecular machines

Recommended books/reference material

1. Ariga, K.; Kunitake, T. *Supramolecular Chemistry-
Fundamentals and Applications Advanced Textbook*,
SpringerVerlag, 2012; 555. ISBN 978-3-540- 26185-8.
2. Hans-Jorg, S. *Applications of Supramolecular Chemistry*, CRC
Press; 2012; 454 p. ISBN: 9781439840146.
3. Jonathan W. Steed, Jerry L. Atwood. *Supramolecular
Chemistry*, 2nd Edition; 2009, John Wiley, ISBN: 978-0-
47051234-0.

Advanced Heterocyclic Chemistry

Course Code: CHM-739

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Comprehend the synthesis, reactivity, and reactions of various heterocyclic compounds.

- Apply knowledge of heterocyclic chemistry to the design and synthesis of complex organic molecules.

Learning Outcomes

- Evaluate the reactivity and synthesis of five- and six-membered heterocycles.
- Synthesize and analyze heterocyclic compounds with multiple heteroatoms and their applications in organic synthesis.

Course Outline

Unit 1. Five-Membered and Six-Membered Rings

Typical reactivity, synthesis, and reactions of pyrroles, thiophenes, furans, pyridines, quinolines, isoquinolines, indoles, benzo[b]thiophenes, benzo[b]furans, isoindoles, benzo[c]thiophenes, isobenzofurans.

Unit 2.

Heterocycles Containing More Than Two Heteroatoms

Reactivity, synthesis, and reactions of 1,3-azoles, imidazoles, thiazoles, and oxazoles. Reactivity, synthesis, and reactions of 1,2-azoles, pyrazoles, isothiazoles, isoxazoles, isoazoles, diazines, pyridazines, pyrimidines, and pyrazines.

Unit 3.

Heterocycles Containing Ring-Junction Nitrogen

Synthesis, reactions, and reactivity of indolizines, aza-indolizines, quinolinizinium and related systems, pyrrolizine and related systems, cyclazines.

Unit 4. Silicon

Organic Compounds Containing Sulfur, Phosphorus, and

Chemistry of sulfur, phosphorus, and silicon compounds including application in organic synthesis.

Unit 5.

Applications and Advanced Topics in Heterocyclic Chemistry

Design and synthesis of complex organic molecules, roles of heterocycles in pharmaceuticals, agrochemicals, and materials science. Case studies and current research trends illustrating cutting-edge applications of heterocyclic compounds.

Recommended books/reference material

1. Finar, I.L. *Organic Chemistry*, 6th Edition; 2009, Vol. I, Pearson Education, Singapore, ISBN: 978-81-7758-542-1.
2. Jacobi, *Introduction to Heterocyclic Chemistry*, 2018 ISBN: 978-1-119-41759-0.
3. Joule, J.A., Mills, K. *Heterocyclic Chemistry*, 4th Edition; 2000, Blackwell Publishing, ISBN: 978-14-0513-300-5.
4. Joule, John, *Heterocyclic Chemistry*, 3rd Edition, 2018, ISBN: 981138455986
5. Scriven, E.F.V., Ramsden, C.A. *Advances in Heterocyclic Chemistry*. Wiley Interscience, 2016, Vol 118, pp 1-314, ISBN: 978-0-12-804696-8.

Advanced Quantum Chemistry

Course Code: CHM-750

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Understand the principles and methods used in the study of manyelectron wave functions and electron correlation.
- Apply advanced quantum chemistry techniques to analyze and solve complex problems in molecular systems.

Learning Outcomes

- Analyze many-electron wave functions and their approximations in quantum chemistry.
- Apply electron-correlation theories to predict and interpret molecular behavior and properties.

Course Outline

Unit 1. Many-Electron Wave Functions

Introduction, Spin orbit interaction, Born-Oppenheimer approximation,

Unit 2. Hartree-Fock Theory

Hartree products, Hartree-Fock approximation, interpretation of solutions of Hartree-Fock equation, restricted closed-shell Hartree-Fock (The Roothaan equation).

Unit 3. Second Quantization: Basics

Creation and annihilation operator and their anticommutation relations, second quantized operators and their matrix elements.

Unit 4.

Second Quantization: Basics

Many particle states and permutation symmetry, completely symmetric and anti-symmetric states, field operators, momentum representation, tensor network and matrix product states, the density matrix renormalization group.

Unit 5. Electron-Correlation Theories

Electron correlation with configuration interaction, perturbation theories, coupled-cluster and Moller-Plesset, quantum chemistry without the Born-Oppenheimer approximation.

Recommended books/reference material

1. Attila Szabo; Neil S. Ostlund. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*; Revised Edition; Dovers; 2005, ISBN13: 080-0759691869.
2. Freeman Dyson. *Advanced Quantum Mechanics*; 2nd Edition; 2011, World Scientific Publishing Company; ISBN-13: 9789814383417.
3. George C. Schatz; Mark A. Ratner. *Quantum Mechanics in Chemistry*; 1st Edition; 2002, Dover Publications; ISBN-13: 978-0486420035.

Advanced Nuclear Chemistry

Course Code: CHM-751

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Understand the principles and techniques used in radiation chemistry and radiochemical processes.
- Apply radiochemical techniques to practical problems, including waste disposal and the use of radiation in various applications.

Learning Outcomes

- Analyze the kinetics and mechanisms of radiation interactions and track etching.

- Apply radiochemical techniques to the synthesis and separation of transuranium and superheavy elements, as well as to the management of radioactive waste.

Course Outline

Unit 1. Introduction to Radiation Chemistry

An introduction to radiation chemistry, kinetics of radioactive decay, kinetics and mechanism of track etching, tracers, production and decay of excited states, energy loss by gamma rays, energy loss by electrons, energy loss of other charged particles, effect of LET, dosimetry, radiolysis of gases, liquids, and solids.

Unit 2. Radiochemical Techniques: Basics

Unique aspects of radiochemistry, recoils, evaporation residues, heavy residues, separation techniques, extraction chromatography, rapid radiochemical separation.

Unit 3. Radiochemical Techniques: Advanced Topics

Transuranium elements, chemistry of transuranium elements, superheavy elements, limits of stability, transuranium elements synthesis, theoretical aspects of reactions.

Unit 4. Reactors and Accelerators

Neutron-induced reactions, neutron-induced fission, de-installation of work-out/old nuclear power plants, charged particle beam transport and analysis, radioactive ion beams.

Unit 5. Radioactive Waste Disposal and Applications

Classification of radioactive wastes, amount and associated hazards, storage and disposal of nuclear wastes. Applications of radiation in radiobiology, sterilizations, polymerization, nitrogen fixation, food preservation, and medicines.

Recommended books/reference material

1. Gregory Choppin; Jan-Olov Liljenzin; Jan Rydberg; Christian Ekberg. *Radiochemistry and Nuclear Chemistry; 4th Edition;*

2013, Academic Press; ISBN13: 978-0124058972. Annexure-14-N, Page 3634 of 3873 Page 50 of 98.

2. Jeffrey I. Steinfeld. *Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy*; 2nd Edition; 2005, Dover Publications; ISBN-13: 978- 0486441528.

3. Marco Montalti; Alberto Credi; Luca Prodi; Teresa Gandolfi. *Handbook of Photochemistry*; 3rd Edition; 2006, CRC Press; ISBN: 13:978-1-4200-1519-5.

4. Walter D. Loveland, David J. Morrissey; Glenn T. Seaborg. *Modern Nuclear Chemistry*; 1st Edition; 2005, Wiley-Interscience; ISBN-13:

978-0471115328.

**Advanced Reaction
Dynamics** Course Code:
CHM-752

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study Reaction dynamics, thermodynamic and kinetic control of reactions.

Learning Outcomes

Students should be able to understand:

- Reaction dynamics, thermodynamic and kinetic control of reactions.
- Theories of reactions rates, unimolecular reactions.
- Kinetics of catalyzed reactions, dynamic and oscillatory reactions.

Course Outline

Unit 1. Introduction to Reaction Dynamics

Molecular reaction dynamics, Microscopic-macroscopic relations, Reaction rate and rate constant, Potential energy surfaces and their influence on reaction pathways.

Unit 2. Theoretical Foundations of Chemical Reactions

Simple collision theory, Modified simple collision theory, Activated complex theory (ACT), Thermodynamic interpretation of ACT.

Unit 3. Unimolecular Reactions and Transition State Dynamics

Dynamics of unimolecular reactions, Lindemann's mechanism, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel-Marcus (RRKM) theory, Marcus treatment of transition states, Kinetic and thermodynamic control, Probing of transition states.

Unit 4. Kinetics of Catalyzed Reactions

Autocatalysis, Enzyme catalyzed reactions, Induced catalysis, Positive catalysis, Negative catalysis, Dynamic chain reactions (e.g., Hydrogen-bromine and Hydrogen-chlorine).

Unit 5. Advanced Topics in Reaction Dynamics

Quantum mechanical treatments of reactions, Transition state theory, Crossing potential energy surfaces, Ultrafast reaction dynamics, Advanced experimental methods in reaction dynamics

Recommended books/reference material

1. John Z. Zhang. (1999) *Quantum Theory & Applications of Chemical Reaction Dynamics*; World Scientific Publishing Company, ISBN-13: 978-9810233884.
2. Paul L. Houston. (2006) *Chemical Kinetics and Reaction Dynamics*; Dover Publications; ISBN-13: 978-0486453347.
3. Peter M. Rentzepis; Christos Capellos. (2012) *Advances in Chemical Reaction Dynamics* (Nato Science Series C); Springer; ISBN-13: 9789401086042.
4. Raphael D. Levine. (2009) *Molecular Reaction Dynamics*; Reprint edition; Cambridge University Press; ISBN-13: 978-0521140713.
5. Fogler, H. S. (2016). *Elements of chemical reaction engineering* (5th ed.). Pearson.

Polymers and Advanced Composite Materials

Course Code: CHM-753

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand:

- Ideal and real polymer chains, kinetics and mechanism of polymerization reactions, Polymers rheology and mechanics, Composite materials, their types, properties and processing of composites.

Learning Outcomes

Students should be able to understand:

- Ideal and real polymer chains, kinetics and mechanism of polymerization reactions.
- Polymers rheology and mechanics.
- Composite materials, their types, properties and processing of composites

Course Outline

Unit 1. Fundamentals of Polymer Chains

Ideal Polymer Chains, Chain conformation and Kuhn model, Free energy, entropy, and elasticity of ideal chains, Fractality of polymers and their structural implications.

Unit 2.

Polymerization Reactions and Mechanisms

Polymerization Reactions, Mechanisms and kinetics of radical, cationic, and anionic polymerization, Polyaddition and polycondensation processes, Rheology, mechanics, and viscoelasticity of polymer systems, Relaxation, creep, and repetition phenomena in polymer melts.

Unit 3.

Estimation of Molecular Weights and Distributions

Molecular Weight Estimation, Fractionation techniques: solubility-based methods, osmometry, light scattering, Size exclusion chromatography for molecular weight analysis and distributions.

Unit 4. Real Polymer Chains and Dynamics

Real Polymer Chains, Interaction potentials and the Mayer function, Conformational dynamics and behavior of real

polymer chains, Factors influencing the dynamics of polymer chains

Unit 5. Composite Materials and Interfaces

Composite Materials, Classification of natural and synthetic composites, Property enhancement through reinforcement and orientation, Interface characteristics and reactions in composite materials, Mechanical and thermal properties of composites, Stress relaxation, creep studies, toughening mechanisms, and mechanical failure in polymeric composites

Recommended books/reference material

1. Charles E. Carraher. (2010), *Introduction to Polymer Chemistry*; 2nd Edition; CRC Press; ISBN-13: 978-1439809532.
2. Chawla; Krishan. (2012) *Composite Materials; Science and Engineering*; ISBN: 978-0387-74365-3.
3. Dan Campbell; Richard A. Pethrick; Jim R. White. (2020) *Polymer Characterization: Physical Techniques*; 3rd Edition; CRC Press; ISBN: 9780748740055
4. Ferrari, A. C., & Giannazzo, F. (Eds.). (2017). *2D materials*. CRC Press.
5. Johnson, Les, and Joseph E. Meany. Graphene: (2018) *the super strong, super thin, and super versatile material that will revolutionize the world*. Prometheus Books

Advanced Statistical Thermodynamics

Course Code: CHM-754

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study partition functions, ensemble theory and methods of statistical thermodynamics

Learning Outcomes

Students should be able to understand:

- Partition functions, ensemble theory and methods of statistical thermodynamics.
- Bose- Einstein, Fermi-Dirac statistics, Einstein and Debye theories for crystalline solids.

Course Outline

Unit 1. Introduction to Ensembles and Partition Functions

Ensembles and distributions in statistical thermodynamics, Canonical ensemble: Definition and properties, Molecular partition function and its interpretation, Translational partition function and its calculation

Unit 2. Calculations of Partition Functions

Rotational and vibrational partition functions, Electronic partition function and its contributions, Ensemble theory and distribution functions, Probability density and ensemble averages of thermodynamic properties

Unit 3. Microcanonical Ensembles and Statistical Methods

Microcanonical ensemble: Definition and characteristics, Statistical methods in thermodynamics, Maxwell-Boltzmann (MB) distribution, System constraints and particle distributions, Microstates, macrostates, and the most probable macrostate

Unit 4. Quantum Statistics and Crystalline Solids

Bose-Einstein and Fermi-Dirac statistics, Stirling's approximation in statistical thermodynamics, Entropy and equilibrium particle distribution, Statistical thermodynamics of crystalline solids, Einstein and Debye theories for thermal properties of solids

Unit 5. Critical Evaluation and Advanced Topics

Critical evaluation of the Debye formulation, Advanced concepts in statistical thermodynamics, Applications in modern physics and chemistry, Emerging trends and research in ensembles and partition functions.

Recommended books/reference material

1. Arieh Ben-Naim. Statistical Thermodynamics with Applications to the Life Sciences; World Scientific Publishing Company; 2014, ISBN-13: 978- 9814578202.
2. Donald W. Rogers. Einstein's "Other" Theory: The Planck-BoseEinstein Theory of Heat Capacity; Princeton University Press; 2005, ISBN-13: 978-0691118260.
3. Leonard K. Nash. Elements of Statistical Thermodynamics; 2nd Edition; 2022, Dover Publications; ISBN-13: 0486137465.
4. Normand M. Laurendeau. Statistical Thermodynamics: Fundamentals and Applications; 1st Edition; 2010, Cambridge University Press; ISBN-13: 978- 0521154192.
5. Stanley I. Sandler. An introduction to Applied Statistical Thermodynamics; 1st Edition; 2010, Wiley; ISBN-13: 978-0470913475. Fried, J. R. (2014). *Polymer science and technology*. (3rd ed.). Prentice Hall. ISBN: 9780137039555

Advanced Solid-State Chemistry and Characterization Techniques

Course Code: CHM-755

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study

- Fractional atomic coordinates, symmetry and Different techniques for characterization of solids

Learning Outcomes

Students should be able to understand:

- Fractional atomic coordinates, symmetry, point and space symmetry.
- Different techniques for characterization of solids: NMR, Diffraction methods, X-ray diffraction and Electron microscopy.

Course Outline

Unit 1. Crystal Structure and Symmetry

Introduction to solid state chemistry, Crystal structure: Types and characteristics.

Fractional atomic coordinates and symmetry elements, Point and space group symmetry, Symmetry operations and their applications, Introduction to quasicrystals and their unique properties.

Unit 2. Electron Microscopy and Spectroscopy

Principles of electron microscopy, Scanning electron microscopy (SEM) and its applications, Electron diffraction spectroscopy (EDS): Techniques and analysis, Transmission electron microscopy (TEM) for imaging and diffraction patterns, X-ray fluorescence spectroscopy (XRF) for elemental analysis, Single particle 3-D reconstruction and its significance.

Unit 3.

Magnetic Resonance Spectroscopy in Solids

Fundamentals of magnetic resonance spectroscopy, Nuclear magnetic resonance (NMR) in solid state: Techniques and applications, Measurement of scalar couplings and their analysis, Measurement of dipolar couplings in NMR, Residual dipolar couplings and their role in structural determination.

Unit 4.

X-ray Diffraction Methods

Introduction to X-ray diffraction (XRD) methods, Single crystal XRD: Analysis of small molecules and macromolecules, Powder XRD: Applications in materials science, Measurement of lattice parameters and defect chemistry, Electrical properties of solids and beta values measurement, Determination of space group and electron density map calculation

Unit 5. Advanced Topics in Solid State Chemistry

Advanced diffraction techniques and their applications, Emerging characterization methods in solid state chemistry, Application of techniques in natural systems and complex materials, Case studies and practical applications in materials science, Future directions and innovations in solid state chemistry research.

Recommended books/reference material

1. Apperley, D. C., Harris, R. K., & Hodgkinson, P. (2012). *Solid state NMR: Basic principles & practice*. Momentum Press. ISBN-13: 9781606503508.
2. Cullity, B. D. (2014). *Elements of X-ray diffraction* (3rd ed.). Pearson. ISBN-13: 978-9332535169.
3. Phillips, P. (2005). *Advanced solid state physics*. Cambridge University Press. ISBN-13: 978-0521523396.
4. Smart, L. E., & Moore, E. A. (2020). *Solid state chemistry: An introduction* (5th ed.). CRC Press. ISBN: 9780429027284.

Advanced Photochemistry and Radiation Chemistry

Course Code: CHM-756

Credit Hours: 3

Pre-requisite: Nil

Objectives

The objective of this course is to study the excited states and photo physical transitions, physical deactivations of excited states and reaction mechanisms.

Learning Outcomes

Students should be able to understand:

- Different energy transfer transition states of electrons, Frank-Condon principle.
- Intersystem crossing, fluorescence, phosphorescence, quenching process.
- Photo electrochemical processes and photo electric cells.

Course Outlines:

Unit 1. Excited States and Photo Physical Transitions

Photon molecule interactions, intensity and strength of electronic transition, selection rules for electronic transition, triplet-triplet, triplet singlet, singlet-triplet energy transfer states.

Unit 2. Multi Photon Energy Transfer Processes

Vibronic states, Franck-Condon principle for phonons, Franck-Condon principle in solvation.

Unit 3. Physical Deactivations of Excited States:

Vibrational relaxations, intersystem crossing, fluorescence,

phosphorescence, quenching process, excited states life times.
Unit 4. Photo Electrochemical Processes & Reactions Mechanisms

Photo excitations, photo isomerization, multi-photon ionization, photo-sensitization, bioluminescence, photodegradation, photo dynamic therapy, photoresist technology,.

Unit 5. Interpretation Of Electronic Spectra

Triple quenching studies, flash photolysis. band gap analysis, band gap and electronic spectra transitions, effects of different bandgaps on photoelectrochemical processes.

Recommended Books/reference material

1. Angelo Albini. Photochemistry: Past, Present and Future; 1st Edition; 2018, Springer; ISBN-13: 978-3662479766.
2. Brian Wardle. Principles and Applications of Photochemistry; 1st Edition; 2010, Wiley; ISBN-13: 978-0470014943.
3. Rachel C. Evans; Peter Douglas; Hugh D. Burrow. Applied Photochemistry, Springer; 2013, ISBN-13: 978-9048138296.

Surface Chemistry

Course Code: CHM-757

Credit Hours: 3

Pre-requisite: Nil

Objectives

The objective of this course is to study Structure, electrical & mechanical properties and thermodynamic aspects of surfaces and different surface analytical techniques.

Learning Outcomes

Students should be able to understand:

- Structure, electrical & mechanical properties and thermodynamic aspects of surfaces.
- Physisorption and chemisorption, different adsorption isotherms.
- Catalytic activity at surfaces and different surface analytical techniques.

Course Outlines:

Unit 1. Structure and Properties of Surfaces

Structure of surfaces, surface chemical bond, electrical and mechanical properties of surfaces thermodynamics of surfaces, dynamics at surfaces.

Unit 2. Adsorption at Surfaces

Physisorption, chemisorption and chemisorbed species, adsorption of gases.

Unit 3. Adsorption from Solutions

Gibb's equation, the extent of adsorption, adsorption Isotherms, Langmuir adsorption isotherm, Freundlich adsorption isotherm, Temkin adsorption isotherm, Brunauer, Emmet and Teller isotherm.

Unit 4. Catalytic Activity at Surfaces

Catalysis by surfaces, catalytic process: hydrogenation, oxidation, cracking and reforming.

Unit 5. Surface Analytical Techniques

Auger electron spectroscopy (AES), photoelectron spectroscopy, X-Ray Photoelectron spectroscopy (XPS)&Ultraviolet Photon Spectroscopy (UPS), secondary ion mass spectroscopy (SIMS), over layer structures & surface diffraction.

Recommended Books/reference materials

1. Gabor A. Somorjai; Yimin Li. Introduction to Surface Chemistry and Catalysis; 3rd Edition; 2020, Wiley; ISBN: 978-0-470-50823-7.

2. Georgios M. Kontogeorgis; Soren Kiil. Introduction to Applied Colloid and Surface Chemistry; Wiley; 2016, ISBN: 978-1-118-88118-7.
3. Hans-Jrgen Butt; Karlheinz Graf; Michael Kappl. Physics and Chemistry of Interfaces; 3rd Edition; 2013, Wiley-VCH; ISBN-13: 978-3527412167.

Magnetic Spin Dynamics

Course Code: CHM-758

Credit Hours: 3

Pre-requisite: Nil

Objectives

The objective of this course is to study the Progress in 1D & 2D NMR and their experimentation.

Learning Outcomes:

Students should be able to understand:

- Advances in 1D & 2D NMR and their experimentation.
- Distortion-less enhancement by polarization transfer, nuclear Overhauser effect.
- Interpretation, quantum mechanical approach & characteristics of NMR spectra.

Course Outline:

Unit 1. One-Dimensional NMR (1D NMR)

Fundamental concepts, types, regular 1D, decoupled, gated decoupled, inverse-gated, 1D NMR experiment, spectral parameters, chemical shift, scalar coupling, interpretation of spectra.

Unit 2. Two-Dimensional NMR (2D NMR)

Fundamental concepts, 2D NMR experiment, types of 2D NMR spectroscopy, methods of 2D NMR

Unit 3. Different Aspects of Correlation Spectroscopy

COSY (Correlation spectroscopy), ECOSY (Exclusive correlation spectroscopy), TOCSY (Total correlation spectroscopy).

Unit 4. Applications of NMR: C-13 NMR

Distortion-less enhancement by polarization transfer, Nuclear Overhauser effect, advances in 1D and 2D-NMR

Spectroscopy, J-resolved,

Unit 5. Quantum Mechanical Description of the NMR Experiment

Characteristics of quadrupolar nucleus—effect of field gradient and magnetic field upon quadrupolar energy levels.

Recommended Books/reference material

1. Alois Steigel; Hans W. Spiess. Dynamic NMR Spectroscopy (NMR Basic Principles and Progress); Springer; 2011, ISBN-13: 978-3642669637.
2. Atta-ur-Rahman; Choudhary Wahab. Solving problems with NMR Spectroscopy; 2nd Edition; 2015, Academic Press; ISBN: 9780124115897.
3. Harald Gunther. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry; 3rd Edition; 2013, Wiley; ISBN: 978-3-52767477-0

Advanced Electrochemistry

Course Code: CHM-759

Credit Hours: 3

Pre-requisite: Nil

Objectives

The objective of this course is to study

□ Different electroanalytical techniques and advances in

Electrochemistry with respect to analytical techniques.

Learning outcomes:

Students should be able to understand:

- Electrode reactions and their kinetics, electrochemical impedance spectroscopy.
- Different electroanalytical techniques, industrial applications of electrochemistry.
- Fuel cells, batteries, semiconductors, different types of sensors.

Course Outline

Unit 1. Electrode Processes

Kinetics of electrode reactions, mass transfer by migration and diffusion, electrochemical potential, electrochemical impedance spectroscopy,

Unit 2. Electrocatalysis

Different types of Electrocatalysis, effects of solution resistance and double layer capacitance, electrode reactions with coupled homogeneous chemical reactions.

Unit 3. Industrial Electrochemistry

Corrosion study, detection, measurement, monitoring and remedies, electro crystallization, energy conversion systems, fuel cells and batteries,

Unit 4. Semiconductor Electrochemistry

Conversion of electrochemical energy in industries, storage of electrochemical energy, capacitors, resistors, types of capacitors and resistors.

Unit 5. Advanced Applications of Electroanalytical Techniques

Potentiometry, coulometry, voltammetry, potential step and potential sweep methods, potentiometric sensors, amperometry and voltametric sensors.

Recommended Books/reference material

1. Allen J. Bard; Larry R. Faulkner. Electrochemical Methods; Fundamentals and Applications; 2nd Edition; 2000, Wiley; ISBN-13: 978-0471043720.
2. Christos Comninellis; Guohua Chen. Electrochemistry for the Environment; Springer; 2009, ISBN-13: 978-0387369228.
3. Derek Pletcher; Zhong-Qun Tian; David Williams. Developments in Electrochemistry: Science Inspired by Martin Fleischmann; Wiley; 2014, ISBN: 978-1-118-69443-5.

4. Keith Oldham; Jan Myland; Alan Bond. Electrochemical Science and Technology: Fundamentals and Applications; Wiley; 2011, ISBN: 978-0470-71084-5.

Advanced Polymer Chemistry

Course Code: CHM-770

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand:

- New classes of advanced polymers and composites as well as new technologies used for processing and for performance applications.
- Polymers into an industrial product by considering the entire process covering monomer synthesis, polymerization chemistry, polymer structure, morphology and process ability.

Learning Outcomes

Upon successful completion of an Advanced Polymer Chemistry course, students should be able to:

- Understand Polymer Structure and Properties
- Describe the chemical structure of various types of polymers, including homopolymers, copolymers, and biopolymers.
- Explain the relationship between polymer structure and physical properties such as crystallinity, melting temperature, glass transition temperature, and mechanical strength.
- Demonstrate proficiency in various polymer synthesis techniques, including free radical polymerization, step-growth polymerization, and living/controlled polymerization methods.
- Utilize modern characterization techniques such as gel permeation chromatography (GPC), nuclear magnetic resonance (NMR) spectroscopy, and differential scanning calorimetry (DSC) to analyze polymer properties.

Course Outline

Unit 1. Polymer Properties& Synthesis

Synthetic routes, Molecular weight (MW), Molecular weight distribution (MWD), chain entanglement, random coil, repetition, crystallinity, viscoelasticity chain growth, step growth, tacticity, carother's equation,

Unit 2. Polymer Characterization and Processing

Gel permeation chromatography (GPC), Mass spectrometry (MS), Differential scanning calorimetry (DSC), Thermogravimetric analysis (TGA), Nuclear magnetic resonance (NMR), Infra-red (IR), Electron spin resonance.

Unit 3. Structure/Property Relationships in Polymers

Glass transition temperature (T_g), Melt temperature (T_m), chemical and thermal stability, viscoelasticity and how these are related to polymer structure (MW, MWD, tacticity etc.), conducting polymers, syntheses of polyacetylenes, polyphenylenes, polyphenylenevinylenes, polyphenylacetylenes, polythiophenes, and polypyrroles.

Unit 4. Conducting Polymers and Their Synthesis

GConducting polymers, synthesis of polyacetylenes, polyphenylenes, polyphenylenevinylenes, polyphenylacetylenes, polythiophenes, and polypyrroles.

Unit 5. Synthetic Strategies for Conjugated Polymer

Nanowire synthesis, examples of electro-active (pseudo) polyrotaxanes, suitable monomers after retrosynthetic analysis, conjugated polymer with particular emphasis on polyacetylenes, polyphenylenes, polyphenylenevinylenes, polyphenylacetylenes, polythiophenes, and polypyrroles.

Recommended books/reference material:

1. Brazel, C. S., & Rosen, S. L. (2012). Fundamental principles of polymeric materials. John Wiley & Sons.
2. Carraher, C. E. (2017). Carraher's polymer chemistry. CRC press.
3. Fried, J. R. (2014). Polymer science and technology. Pearson Education.

- Koltzenburg, S., Maskos, M., & Nuyken, O. (2017). Polymer chemistry. Springer.
4. Koo, J. H. (2019). Polymer nanocomposites: processing, characterization, and applications. McGraw-Hill Education.
 5. Nicholson, J. (2017). The chemistry of polymers. Royal Society of Chemistry.
 6. Schröder, H. V., & Schalley, C. A. (2019). Electrochemically switchable rotaxanes: recent strides in new directions. Chemical Science, 10(42), 9626-9639.

Physical Structure of Porous Materials

Course Code: CHM-771

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand:

- The working principles and conditions of various electron microscopic techniques for materials characterization.
- Material characterization techniques.

Learning Outcomes

Upon successful completion of course, students should be able to:

- Describe the basic concepts and definitions related to porous materials, including porosity, pore size distribution, and specific surface area. □ Identify different types of porous materials (e.g., microporous, mesoporous, macroporous) and their structural characteristics
- Utilize various techniques to characterize the physical structure of porous materials, such as gas adsorption, mercury intrusion porosimetry, and scanning electron microscopy (SEM).
- Analyze and interpret data obtained from characterization techniques to determine pore size distribution, surface area, and porosity. □ Describe common methods for the synthesis and fabrication of porous materials, including templating, sol-gel processes, and hydrothermal synthesis.
- Explain how synthesis parameters influence the structural properties of porous materials.

Course Outline

Unit 1. Electron Microscopy Techniques

Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Scanning Transmission Electron Microscopy (STEM), Energy Dispersive X-Ray Analysis (EDX), and Electron Energy Loss Spectroscopy (EELS).

Unit 2. Material Characterization Techniques

Molecular symmetry, basic crystallography, band theory, porous materials, nano-structured materials and some material characterization techniques including powder X-Ray diffraction and physical adsorption, gas adsorption and various spectroscopic methods of analysis, especially FT-IR and solid-state NMR.

Unit 3. Synthesis and Fabrication Methods for Porous Materials

Porous materials are characterized by their high surface area and pore volume, making them suitable for a variety of applications such as catalysis, adsorption, and separation. The synthesis and fabrication methods for porous materials are diverse and can be tailored to achieve specific pore sizes and structures. Here are some common methods, Template Synthesis, Hydrothermal and solvothermal synthesis

Unit 4. Sol-Gel Process

The sol-gel process involves the transition of a solution (sol) into a solid gel phase. Hydrolysis and polycondensation of metal alkoxides or inorganic salts to form a colloidal suspension. Gelation of the sol to form a network structure. Drying and aging to remove the solvent and strengthen the gel. Calcination to remove organic residues and enhance porosity. Application: Used to synthesize silica, alumina, and other metal oxides with controlled pore sizes.

Unit 5. Other Methods of Synthesis

Template Synthesis: Hard Templating (Nanocasting), Uses solid templates like silica or carbon, which are later removed by chemical etching or calcination. Soft Templating: Utilizes surfactants or block copolymers that form micelles or liquid crystalline phases, which guide the material structure.

Applications: Used for synthesizing mesoporous materials like MCM-41, SBA-15, and mesoporous carbons. Hydrothermal and Solvothermal Synthesis: Mixing the precursors in a solvent. Sealing the mixture in an autoclave. Heating the autoclave to initiate the crystallization of the porous material. Cooling and recovering the porous product. Applications: Commonly used for the synthesis of zeolites, metal-organic frameworks (MOFs), and other crystalline porous materials.

Recommended books/reference material:

1. Bennett, T. D., Coudert, F. X., James, S. L., & Cooper, A. I. (2021). The changing state of porous materials. *Nature Materials*, 20(9), 1179-1187. Elsevier.
2. Goldstein, J. I., Newbury, D. E., Michael, J. R., Ritchie, N. W., Scott, J. H. J., & Joy, D. C. (2017). *Scanning electron microscopy and X-ray microanalysis*. Springer
3. Hübschen, G., Altpeter, I., Tschuncky, R., & Herrmann, H. G. (Eds.). (2016). *Materials characterization using nondestructive evaluation (NDE) methods*. Woodhead publishing.
4. Liu, P. S., & Chen, G. F. (2014). *Porous materials: processing and applications*.
5. Van Der Voort, P., Leus, K., & De Canck, E. (2019). *Introduction to Porous Materials*. John Wiley & Sons.

Agrochemicals

Course Code: CHM-772

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand:

- The factors involved in the discovery of different fertilizers.
- Development of modern agrochemicals.

Learning Outcomes

Upon Successful Completion of the Agrochemicals Course, Student be able to understand:

- Identify and describe the various types of agrochemicals, including pesticides, herbicides, fungicides, fertilizers, and plant growth regulators.
- Explain the specific applications and benefits of each type of agrochemical in modern agriculture.
- Understand the chemical structures, properties, and modes of action of commonly used agrochemicals.
- Describe how agrochemicals interact with target organisms and plants at the molecular level.

Course Outline

Unit 1. Manures

Sources and production of manures, different composting technologies- mechanical compost plants, vermi composting- green manures–oil cakes-sewage sludge-biogas plant slurry-plant and animal refuges.

Unit 2. Fertilizers Classification

Manufacturing of ammonium sulphate, ammonium chloride, ammonium nitrate and urea, phosphatic fertilizers: p fertilizer sources–processing rock phosphate, bones for bone meal preparation–basic slag–preparation of single, triple super phosphate and thermo-phosphate.

Unit 3. Potassic Fertilizers

K fertilizer, natural sources, manufacturing of KCl, potassium sulphate and potassium nitrate.

Unit 4. Mixed and Complex Fertilizers

Sources and compatibility, preparation of major, secondary and micronutrient mixtures, complex fertilizers, manufacturing of ammonium phosphates, nitro phosphates and NPK complex, biofertilizers and their advantage-fertilizer control order and fertilizer storage, organic chemistry as prelude to agrochemicals.

Unit 5. Herbicides–Fungicides

Manures, green manures, oilcakes, sewage sludge, biogas plant slurryplant and animal refuges, p-fertilizers, rock phosphate, bone meal, single and triple super phosphates–

thermosphosphates– method of manufacturing, potassic fertilizers–manufacturing of KCl, K₂SO₄ and schoenite. Secondary and micronutrient fertilizers: Manufacturing zinc sulphate and ferrousulphate, complex fertilizers and ammonium phosphates–nitro phosphates and NPK complexes.

Recommended books/reference material:

1. Bockman, O. C., Kaarstad, O., Lie, O. H., & Richards, I. (2015). Agriculture and fertilizers. Scientific Publishers. ButterworthHeinemann.
2. Chojnacka, K., & Saeid, A. (Eds.). (2021). Smart Agrochemicals for Sustainable Agriculture. Academic Press.
3. Havlin, J.L., Tisdale, S.L., Nelson, W.L., Beaton, J.D. Soil Fertility and Nutrient Management: An Introduction to Nutrient Management, 8thEdition; 2014, Pearson, ISBN: 0130278246.
4. Montgomery, J. H. (2020). Agrochemicals desk reference. CRC Press.
5. Prasad, M. N. V. (Ed.). (2020). Agrochemicals detection, treatment and remediation.

Industrial Process Chemistry

Course Code: CHM-773

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand:

- Unit operation of coal and ores industries.
- Size and density separation processes

Learning Outcomes

Upon Successful Completion of the Course, Student be able to understand:

- Describe the fundamental principles of industrial process chemistry, including reaction mechanisms, thermodynamics, and kinetics.
- Explain the role of catalysis and the importance of reaction conditions in industrial chemical processes.
- Identify and explain the key steps involved in major industrial chemical processes, such as those for the production of ammonia, sulfuric acid, ethylene, and polymers.

- Analyze process flow diagrams and understand the sequence of operations in industrial chemical manufacturing.
- Apply principles of chemical engineering and process design to develop and optimize industrial chemical processes.
- Use computational tools and simulation software to model chemical processes and predict performance under various conditions.

Course Outline

Unit 1. Economic and Industrial Minerals

Types, occurrence and distribution, basic characterization concepts, overview of separation processes, mineral processing techniques.

Unit 2. Crushing and Grinding

Concept of mineral liberation, characterization of particles, size distributions, the importance of crushing and grinding in the liberation of ores.

Unit 3. Separation of Particles by Size

Screening, classification, hydro cyclones, particle separation based on mineral properties, gravity separation, dense media separation, magnetic and electrostatic separation, separation based on mineral surface properties, froth depressants, collectors, frothers, flotation equipment.

Unit 4. Physical Separation of Slurries

Dewatering of mineral slurries, thickening, filtration, centrifuges, tailings disposal, examples of plant layout and circuit design, copper leaching, gold cyanidation, environmental and safety issues.

Unit 5. Characterization of Industrial Processes

Flow Diagrams: Create detailed process flow diagrams (PFDs) and piping and instrumentation diagrams (P&IDs) to visualize the sequence of operations, equipment, and control systems. Material Balances: Calculate material balances to account for the input and output of materials, ensuring mass conservation throughout the process. Energy Balances: Perform energy balance calculations to analyze energy

consumption, heat generation, and heat losses, optimizing thermal efficiency.

Recommended books/reference material

1. Harmsen, J., & Powell, J. B. (2010). Sustainable development in the process industries. Hoboken, NJ: John Wiley & Sons.
2. Holdich, R. (2020). Fundamentals of particle technology. Midland IT.
3. Kletz, T. (2018). HAZOP and HAZAN: identifying and assessing process industry hazards. CRC Press.
4. PE, D. L. E. (2014). Industrial chemical process design. McGraw-Hill Education.
5. Tripathy, S. K., Banerjee, P. K., Suresh, N., Murthy, Y. R., & Singh, V. (2017). Dry high-intensity magnetic separation in mineral industry—a review of present status and future prospects. Mineral Processing and Extractive Metallurgy Review, 38(6), 339365.

Coal gas and liquefaction

Course Code: CHM-774

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students will acquire the ability to produce synthetic oil and convert coal into liquid fuel.

Learning Outcomes

Students should be able to understand:

- To convert coal into liquid fuels either by removal of carbon or addition of hydrogen.
- To produce synthetic oil to supplement the natural sources of petroleum.

Course Outline

- Unit 1.** **Historical Developments in Coal Liquefaction**
- Historical overview of coal liquefaction, Early coal liquefaction processes: Pott and Broch Process, Bergius Process.
- Unit 2.** **Solvent Extraction of Coal**
- Overview of solvent extraction, Experimental studies on solvent extraction, Mechanism of solvent extraction, Types of solvent extraction, Solvent systems, Supercritical gas extraction, Commercial solvent extraction processes: SRC-I, SRC-II, EDS, Supercritical Gas Extraction
- Unit 3.** **Direct Liquefaction of Coal**
- Direct liquefaction through catalytic hydrogenation, Mechanism of direct liquefaction, Catalyst systems and roles, Catalyst poisoning and management, Catalytic role of coal minerals, Commercial catalytic hydrogenation processes: H-Coal Process
- Unit 4.** **Indirect Liquefaction of Coal**
- Indirect liquefaction methods: Fischer-Tropsch Synthesis, Methanol Synthesis, MTG (Methanol to Gasoline) Processes, Effect of parameters on liquefaction: Coal properties (rank, maceral components, mineral matter) Operating conditions (temperature, pressure, residence time, solvent, catalyst)
- Unit 5.** **Processing of Coal Liquids and Environmental Aspects**
- Purification of liquefaction products, Solid separation and fractionation, Upgrading and characterization of coal-derived liquids, Properties of coal-derived liquids, Liquefaction reactors: Description of high-pressure coal liquefaction reactors, Auxiliary devices, Ebullated bed reactor, Fluidization, Environmental considerations: Air emissions, Water effluents, Solid waste disposal.

Recommended books/reference material

1. Yürüm, Y. (Ed.). (2013). *Clean utilization of coal: Coal structure and reactivity, cleaning and environmental aspects* (Vol. 370). Springer Science & Business Media.
2. Lee, S., Speight, J. G., & Loyalka, S. K. (Eds.). (2014). *Handbook of alternative fuel technologies*. CRC Press.
3. Riazi, M. R., & Gupta, R. (Eds.). (2015). *Coal production and processing technology*. CRC Press.
4. Botsaris, G. D., & Glazman, Y. M. (2022). *Interfacial phenomena in coal technology*. CRC Press.
5. Qyyum, M. A., Chaniago, Y. D., Ali, W., Qadeer, K., & Lee, M. (2019). Coal to clean energy: Energy-efficient single-loop mixed-refrigerantbased schemes for the liquefaction of synthetic natural gas. *Journal of Cleaner Production*, 211, 574-589.

Environmental Impact of Chemical Industries

Course Code: CHM-775

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is

- To study Environmental Impact of Chemical Industries

Learning Outcomes

Students should be able to understand:

- The wide range of environmental regulations and permitting requirements for hazardous materials, waste stream management, air quality, water quality and hazardous materials transportation.
- About the skills to protect the environment and avoid unnecessary liability.

Course Outline

Unit 1. Environmental Management

Environmental management, environmental, health and safety, emergency management, environmental management for industry and facilities, environmental regulations and permitting requirements for hazardous materials, waste stream

management, air quality, water quality and hazardous materials transportation, sustainable best practices, protect the environment and avoid unnecessary liability.

Unit 2. Environmental regulations

Environmental regulations, laws and policies, government air quality framework (GAQF) from the legal and regulatory perspective, health and environmental impacts of chemical hazards, hazardous waste transportation, water quality regulations and the federal clean water act, environmental management and sustainability. environmental impact assessment (EIA), EIA of petrochemical, metal, mining, food, agriculture, pulp and paper industries on air, water, land, and human being.

Unit 3. GIS and RS of pollutants released

Pollution control technologies, assessing environmental impact on lakes, streams and oceans, global warming, climate action and mitigation measures, carbon sequestration and carbon tax.

Recommended books/reference material

1. Glasson, J., & Therivel, R. (2013). *Introduction to environmental impact assessment*. Routledge.
2. Manahan, S. (2017). *Environmental chemistry*. CRC press.
3. Hussain, C. M., & Kecili, R. (2019). *Modern environmental analysis techniques for pollutants*. Elsevier.
4. Wypych, G. (Ed.). (2019). *Handbook of Solvents, Volume 2: Use, Health, and Environment*. Elsevier.
5. Hanif, M. A., Nadeem, F., Bhatti, I. A., & Tauqeer, H. M. (2020). *Environmental Chemistry: A Comprehensive Approach*. John Wiley & Sons
6. Hussain, C. M. (2020). *The handbook of environmental remediation: classic and modern techniques*. Royal Society of Chemistry.

Enzymes Kinetics

Course Code: CHM-790

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study the binding modes between enzymes substrates, inhibitors and enzymes patterns. They will also study their pharmaceutical applications.

Learning Outcomes

- The different binding modes between enzyme, Substrate, Inhibitor and enzymes pattern in different diseases of heart and liver.
- Pharmaceutical applications of enzymes in drug design process.

Course Outline

Unit 1. Enzyme Models

The Michaelis-Menten equation, Lineweaver-Burk plot, Positive and negative cooperatively.

Unit 2. Enzyme Kinetics

The steady-state assumption, derivation of velocity equations from models, fitting of data by non-linear regression. Dissociation constants of substrates and inhibitors.

Unit 3. Enzyme Inhibitors

Inhibition patterns, competitive, noncompetitive and uncompetitive inhibition, tight-binding inhibitors, slow tight-binding inhibitors, enzyme pattern in diseases, myocardial infarction, cardiac troponins, enzymes estimation in serum for diagnosis of muscle, liver and cancer enzymes.

Unit 4. Enzyme Inhibitors as Drugs

Mechanisms of drug resistance, assays for kinetic analysis of enzymes, measurement of initial reaction velocities, chirality and enzymes, prochiral substrates (aconitase), D-Form of human immunodeficiency virus (HIV) protease.

Unit 5. Regulation of Enzymes

Zymogens (chymotrypsinogen) and activation of latent enzymes, competitive inhibitors, bovine pancreatic trypsin inhibitor (BPTI), protein conformation and regulation, intrasteric control, allosteric regulation, glycogen phosphorylase, feedback and metabolic control, enzyme degradation and compartmentation of metabolic pathways..

Recommended Books/reference material

1. Pei, L., & Schmidt, M. (2019). Novel biotechnological approaches to produce biological compounds: challenges and opportunities for science communication. *Current opinion in biotechnology*, 56, 43-47.
2. Bhatia, S., & Bhatia, S. (2018). Introduction to enzymes and their applications. *Introduction to pharmaceutical biotechnology*, 2, 1-29.
3. Alberty, R. A. (2011). Enzyme kinetics: rapid-equilibrium applications of Mathematica.
4. Naghavi, N. S., Sanei, N., & Koller, M. (2022). Enzyme Immobilization and Its Application Strategies in Food Products. In *Novel Food Grade Enzymes: Applications in Food Processing and Preservation Industries* (pp. 411-438). Singapore: Springer Nature Singapore.
5. Garske, A. L., Kapp, G., & McAuliffe, J. C. (2017). Industrial enzymes and biocatalysis. *Handbook of industrial chemistry and biotechnology*, 1571-1638.

Drug-Protein and Drug-DNA Interaction

Course Code: CHM-791

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study drugs, proteins and their applications

Learning Outcomes

- Students will have understanding of different binding modes between drugs and proteins and DNA, awareness about new technologies for the determination of Drug-DNA/protein Interactions.
- How to apply these advanced concepts in the research to strengthen pharmaceutical application of particular synthesized drug molecule in coping diseases at preliminary stages

Course Outline

Unit 1. Drug-protein Interaction

Intracellular and extracellular bindings, prediction of non-bonding interactions in drug design, G-protein coupled receptors, Theories for drug-protein interactions, Ligand binding theory, Topographical, Stereochemical considerations.

Unit 2. Determination of Drug-Protein Interactions:

Fluorometric assays, fluorescence labels, fluorescence correlation spectroscopy, surface plasmon resonance.

Unit 3.

Determination of Drug-DNA Interactions:

Spectroscopic methods of analysis including HNMR spectrum of oligonucleotides, nuclear overhauser enhancement spectroscopy (NOESY) and correlation spectroscopy (COSY) spectra, solution conformation, covalent drug binding, ¹⁹⁵Pt NMR, heteronuclear single quantum coherence spectroscopy (HSQC) experiments, reversible drug binding, circular dichroism, synchrotron radiation circular dichroism, linear dichroism, film LD, interaction between metal complex, duplex DNA & quadruplex DNA.

Unit 4.

Probing DNA and RNA Interactions with Biogenic and Synthetic Polyamines:

Analytical methods used for structural analysis of polyaminesnucleic acid complexes, FTIR spectroscopy, absorption spectroscopy, capillary electrophoresis, molecular modeling, and circular dichroism (CD) spectra.

Unit 5.

Theories for drug-receptor interactions:

The time course of changes in receptor occupancy, partial agonists, inhibitory actions at receptors, topographical and stereo chemical considerations.

Recommended books/reference material

1. Alasdair, J. G, John, C. F. Torben, H. (2011). *Textbook of Receptor Pharmacology*, CRC press. Taylor & Francis group: ISBN: 9781420052541.
2. Boham, H. J, Scheinder, G. (2005) *Protein Ligand Interaction: From Molecular Recognition to Drug Design*, Wiley VCH: Vol. 20.
3. Harvey, R. A, Ferrier, D. R, Karandish, S. (2010) *Lippincott's Illustrated Reviews: Biochemistry, Biochemistry Map (Med Maps) Bundle*, 5thEdition; Lippincott Williams & Wilkins: ISBN: 9781451116311.
4. Keith, R. F. (2010) *Drug-DNA Interaction Protocol*, Springer. ISBN: 9781607615194.
5. Murray, R. M, Harper, H. A. (2000) *Harper's Biochemistry*, 25thEdition; Appleton & Lange: ISBN: 9780838536841.

Bioinformatics

Course Code: CHM-792

Credit Hours: 03

Pre-requisite: Nil

Objectives

- To provide a comprehensive understanding of the fundamental principles and applications of bioinformatics in analyzing biological data.
- To equip students with the skills and tools necessary to perform computational analysis of DNA, RNA, and protein sequences, and to predict their structure and function.

Learning Outcomes

- Students will be able to explain the historical development, uses, and fundamental principles of bioinformatics, as well as compare its applications with experimental tools.
- Students will be proficient in utilizing bioinformatics databases and computational tools to analyze and interpret biological sequences, and predict their structural and functional properties.

Course Outline

Unit 1. Introduction to Bioinformatics (BI)

What is BI? History of BI, Uses of BI (Protein, Gene), Comparison of BI with experimental tools.

Unit 2. Basic Principles of Computing in Bioinformatics

Basic acquisition and database, DDBJ, NCBI, and EMBL.

Unit 3.

Enzyme Classification and Sequence Analysis

Enzyme classification: Retrieval databases, Short introduction to DNA, RNA, and protein, amino acids, sequence, Analyzing protein sequence by the use of BI tools, Sequence-structure function, Retrieving protein sequences from database (FASTA).

Unit 4.

Sequence Alignment and Structure Prediction

Alignment of protein/nucleotide sequences (BLAST, CLUSTALW), Computing physicochemical parameters of proteins (e.g. PROTPARAM), Predicting elements of secondary structure of proteins (e.g. PSSP), Retrieval, understanding, and predicting 3D structure of protein from sequence, Posttranslational modifications (e.g. NETPHOS, etc.).

Unit 5. DNA/RNA Analysis and Primer Designing

Short introduction to DNA/RNA: Structure, genetic code, Analyzing DNA/RNA sequence by the use of BI tools, Retrieving DNA sequence from database, Computing the sequence, Identifying restriction sites, Predicting elements of DNA/RNA secondary structure, Computing the optimal alignment between two or more DNA sequences, PRIMER Designing for PCR: PRIMER3+, PRIMER BLAST, OLIGO-CALC, etc. Short introduction to Proteomics and Genomics, Role of bioinformatics in the pharmaceutical industry.

Recommended books/reference material

1. Lesk, A. M. (2019). *Introduction to Bioinformatics* (5th ed.). Oxford University Press.
2. Mount, D. W. (2004). *Bioinformatics: Sequence and Genome Analysis* (2nd ed.). Cold Spring Harbor Laboratory Press.
3. Pevsner, J. (2015). *Bioinformatics and Functional Genomics* (3rd ed.). Wiley-Blackwell.

Clinical Biochemistry

Course Code: CHM-793

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students will acquire teaching and technical capabilities in pharmaceutical, clinical laboratory and professional life as well.

Learning Outcomes

Students should be able to understand:

- The scope of enzymes in diagnosis and monitoring of heart, liver and kidney diseases.
- Acquire teaching and technical capabilities in pharmaceutical, clinical laboratory and professional life as well.

Course Outline

- Unit 1. Enzymes in Diagnosis and Monitoring**
- Role of enzymes in clinical diagnostics, Enzymes in myocardial infarction: Creatine Kinase (CK), Troponin T, Lactate Dehydrogenase (LDH), Normal and abnormal serum values: Interpretation and significance, Enzymes in liver diseases: Serum Glutamic-Oxaloacetic, Transaminase (SGOT), Serum Glutamic-Pyruvic Transaminase (SGPT), Acid and Alkaline Phosphatase, Enzymes in pancreatic diseases: α -Amylase, Normal and abnormal serum values: Diagnostic relevance
- Unit 2. Blood Chemistry and Its Clinical Significance**
- Normal and abnormal blood constituents: Glucose, Urea, Uric Acid, Creatinine, Bilirubin, Proteins, Lipid profile: LDL, HDL, Total cholesterol, Triglycerides, Blood group systems: A, B, AB, O, Rhesus factor (Rh) and transfusion compatibility, Hemoglobinopathies: Anemia, Thalassemia, Sickle Cell Anemia
- Unit 3. Liver Diseases and Their Biochemical Assessment**
- Types of jaundice: Pre-hepatic, Hepatic, Post-hepatic, Biochemical differentiation of jaundice, Liver diseases: Viral hepatitis, Alcoholic hepatitis, Cirrhosis, Molecular basis and biochemical assessment
- Unit 4. Cardiac Diseases and Diagnostic Techniques**
- Cardiac diseases: Ischemic heart disease, Angina pectoris, Myocardial infarction, Diagnostic tests and cardiac profile, Atherosclerotic plaques: Biochemical markers and imaging techniques Non-invasive diagnostic techniques: Sonography, X-ray, MRI, CT scan, Electrocardiogram (ECG): Interpretation and clinical significance
- Unit 5. Cancer, Genetic Disorders, and Infectious Diseases**

Cancer: Molecular basis, Carcinogenesis, Oncogenes, Benign vs. Malignant, Metastasis, Tumor markers, Tumor staging, Genetic disorders: Down syndrome, Turner syndrome, Klinefelter syndrome, Infectious diseases: AIDS, SARS, Dengue, Inborn errors of metabolism, Metabolic disorders, Diabetes

Recommended books/reference material

1. Alberts, B. (2008). *Molecular biology of the cell* (5th ed.). Garland Science. ISBN: 9780815341116. (Annexure-14-N, p. 3682 of 3873).
2. Arthur, R. S. (2009). *Enzyme kinetics: From diastase to multi-enzyme systems*. Cambridge University Press. ISBN: 978-051160843-8.
3. Berg, J. M., Tymoczko, J. L., Gatto, G. J., & Stryer, L. (2015). *Biochemistry* (8th ed.). W. H. Freeman. ISBN-13: 978-1464126109.
4. Voet, D., & Voet, J. D. (2011). *Biochemistry* (4th ed.). John Wiley & Sons. ISBN: 0470917458, 9780470917459.
5. Campbell, M. K., & Farrell, S. O. (2017). *Biochemistry* (9th ed.). Cengage Learning.

Course Title: Biosensors

Course Code: CHM-794

Credit Hours: 3

Prerequisite: Nil

Objectives:

The objectives of this course is to study the types & applications of biosensors regarding environment, medicine, agriculture fields and in the form of electrical appliances

Course Outcomes:

Students should be able to understand:

- The types & applications of biosensors regarding environment, medicine, agriculture fields and in the form of electrical appliances.
- The laws in deducing signal transduction

Course Outline:

Unit.1. Biosensor Applications and Issues

Medicine, agriculture, bioproduction and environment, desired characteristics of biosensor, reliability, simplicity, cost, and related parameters, Operating conditions, Calibration, positive and negative controls and safety measures.

Unit 2.

Biochemical Recognition

Chemical reactions, problems of specificity, plant lectins, biochemical properties and their use in the detection of organism specific polysaccharides. Enzymes: Biological catalysts, specificity, activity, storage/shelf life, enzyme kinetics in solution and on a surface, chemical equilibria-forcing an unfavorable reaction.

Unit 3.

Cells

Signal transduction through chemoreception, membrane potential, cell metabolism and cytotoxicity.

Unit 4.

Antibodies

Immunochemistry, binding affinity and kinetics complementary nucleic acid sequences (RNA and DNA).

Unit 5.

Common Assaying Formats

Radioisotopes, fluorophores, dyes, enzymes/substrates, liposomes, enzyme-linked immunosorbent assay (ELISA's) and nucleotide capture assays, immobilization of biochemical recognition element and conjugation of labels.

Unit 6.

Optical Sensors

Optics-sources (LEDs, lasers, lamps), detectors (photodiodes, photomultiplier tubes, charge coupled devices) and circuits (filters, gratings, fiber optics), detection of absorbance, reflectance and fluorescence, Surface Plasmon Resonance (SPR) based devices.

Recommended books:

- Cass, T., Cooper, J. Biosensors (Practical Approach Series), 2nd Edition; 2004, Oxford University Press: ISBN: 0-19-963846-2.
- Eggins, B.R. Chemical Sensors and Biosensors, John Wiley and Sons, 2003, ISBN: 0471-899-14-3.
- Lucas, L.J. Introduction to Biosensors, Springer-Verlag: New York, 2012, ISBN: 144196021X.
- Marks, R.S; Cullen, D.C; Karube, I. Handbook of Biosensors and Biochips, Wiley: 2014, ISBN: 9780470061565.
- Sadana, A; Sadana N. Handbook of Biosensors and Biosensor Kinetics, Taylor & Francis: 2011, ISBN: 978-0-444-53262-6.

Cell Biology

Course Code: CHM-795

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study cell biology.

Learning Outcomes

Students should be able to understand:

- The role of cell organelles in signaling & signal transduction pathways.
- The degradation of cells and fundamentals of cancerous cells and helped in understanding the treatment therapies of carcinogenic diseases.

Course Outline

Unit 1. Cell Biology

Technical aspects and approaches (i.e. tools of the trade) protein synthesis & transport into organelles vesicular traffic-exocytosis & endocytosis mitosis & molecular regulation of the cell cycle, the cytoskeleton.

Unit 2.**Cell Adhesion and Cell Motility**

The cytoskeleton and the cell surface microtubules and mitosis intermediate filaments actin and myosin muscle contraction & cell motility cell junctions, Cell adhesion and extracellular.

Unit 3. Intercellular Signaling

Hydroformylation, Membrane function and signal transduction structure, composition and properties of biological membranes membrane proteins and transport cell signaling & signal transduction.

Unit 4. Cell Biology in Context

Neurons, cancer and stem cells, membrane transport and neural communication, molecular basis of cancer and cancer cell behavior, stem cells engineering and ethics of stem cell therapy.

Recommended books/reference material

1. Alberts, B; Bray, D; Hopkin, K; Johnson, A; Lewis, J; Raff, M; Roberts, K; Walter, P. (2014), *Essential cell biology*, (4th Ed.); Garland Science Taylor and Francis group, ISBN: 978-0-81534454-4.
2. Guyton, A. C; Hall, J. E; Guyton, Hall. (2011), *Textbook of medical physiology*, (12th Ed.), Saunders Elsevier: ISBN-13: 978-1416045748.
3. Nelson, D.L. (2008), *Lehninger's Principles of Biochemistry*, (6th Ed.); Macmillan Higher Education: ISBN: 9781429222631.

Course Title: Industrial Microbiology

Course Code: CHM-796

Credit Hours: 3

Objectives

Students should be able to understand:

- The scope of fermentation process on industrial and pharmaceutical level.
- The role of mutants in developing quality control products keeping in view the environmental hazards.

Course Outline:

Unit 1. Industrial Microbiology and Biotechnology

Multidisciplinary nature, obsolescence of procedures and methods, organizational set-up in an industrial microbiology establishment, upstream processing (USP) and downstream processing (DSP), unit downstream processing.

Unit 2. A Typical Bioprocess

Advantages and limitations, industrial fermentation products and their producer microorganisms, patents and intellectual property rights, scope of industrial microbiology.

Unit 3. Industrial Microorganisms

Taxonomic diversity of industrially useful bacteria and fungi, characteristics important in microbes used in industrial microbiology and biotechnology, isolation of suitable producer microorganisms from the environment, concept and examples of microorganisms classified as generally recognized as safe (GRAS), culture collections of industrially important microorganisms, industrial producer strains and strain improvement (outline and importance of the process).

Unit 4. Product Development, Regulation and Safety

Development of a pharmaceutical product, product quality and safety (quality assurance components), manufacturing and environmental safety.

Unit 5. Foundation for Calculations in Bioprocess Engineering

Physical variables, dimensions and units (substantial variables, natural variables, dimensional homogeneity in equations, equations without dimensional homogeneity), units, force and weight, measurement conventions (density, specific gravity, specific volume, mole, chemical compositions, temperature and pressure), standard conditions and ideal gases, physical and chemical property data, stoichiometry, area/volume calculations.

Recommended books/reference material

1. Alberts, B. Molecular Biology of the Cell, 5th Edition; 2008, Garland Science: ISBN: 9780815341116.
2. Michael, J.W; Neil, L.M; John, S.R; Gary, H. Industrial Microbiology: An Introduction, 2nd Edition; 2001, Blackwell Scientific, ISBN: 0-632-05307-0.
3. Robert, A.C. Enzymes: A Practical Introduction to Structure, Mechanism, and Data Analysis, 2nd Edition; 2000, John-Wiley & Sons: ISBN: 0-47135929-7.
4. Shankara, Y.M.S. Laboratory Manual for Practical Biochemistry, 1st Edition; 2008, Jaypee Brothers Medical Publishers: India, ISBN: 97881-8448-259-1

Nutraceutical Tissue Culture Technique

Course Code: CHM-797

Credit Hours: 03

Objectives

By studying this course, students should be able to understand the scope of genetic engineering in food technology. The treatment of carcinogenic diseases by plant phenolic, fatty acids and probiotics using novel fermentation and stabilization technologies.

Learning Outcomes

- Students will have understanding of genetic engineering in food technology.
- They will be able to treat carcinogenic disorders by plant phenolic, fatty acids and probiotics by using novel technologies like fermentation and stabilization.

Course outline

Unit 1. Overview of Diet-Gene Interactions and Role of Xanthophylls

Diet-gene interaction in human disease, xanthophylls and their synergism with other dietary factors in human health-protection against eye disease and other chronic diseases, dietary sources of zeaxanthin and lutein and their potential enhancement. Therapeutic potential of dietary polyphenols, curcumin, tocopherol and tocotrienols, limonene, allicin and diallyl disulfide, caffeic acid phenethyl ester, ethyl ferulate, epigallocatechin-3-gallate.

Unit 2.

Nutraceutical Use of Garlic Sulfur-Containing Compounds

Garlic chemical compounds, garlic biological activities, alliin and allicin, garlic alliinase, garlic hydroxides, layered double hydroxides, alginates. Plant phenolics in the prevention and treatment of cancer, epidemiology of plant foods and disease incidence, anticancer phytochemicals, classification and occurrence, cellular mechanisms modified by plant phenolics that can reduce carcinogenesis and tumour progression.

Unit 3. Endogenous Antioxidants and Radical Scavengers

Endogenous antioxidant molecules, reactive oxygen species, reducing disease and obesity risks. The zone diet nutrition strategy, dietary phytochemicals and human health. Crotenoids, phenolic compounds, phytoestrogens, polyunsaturated fatty acids, conjugated linoleic acids, tocopherols and tocotrienols. Limonene, allicin and diallyl disulfide, glucosinolates, capsaicinoids.

Unit 4. Genetic Engineering to Enhance Crop-Based Phytonutrients

Diet and human diseases, phytonutrients and antiproliferative activity. Genetic engineering to improve nutrients, proteins and amino acids, folates, carotenoids, vitamin C and polyphenolics, plants and microalgal chloroplast. Application to food technology, biological elicitors of plant secondary metabolites, defence responses in plants, perceptions and transduction of general elicitors. Techniques to improve secondary metabolite production, elicitor signaling pathways.

Recommended books/reference material

1. Giardi, M.T., Rea G., Berra, B. (2010), *Bio-Farms for Nutraceuticals: Functional Food and Safety Control*, By Biosensors, Springer Landes Bioscience: USA, ISBN: 978-14419-7346-7.
2. Bettina, S. (2009), *Nursing and Clinical Informatics: Socio-Technical Approaches*, Medical Information Science Hershey: New York, ISBN: 978-1-60566-234-3.
3. Lockwood, B. (2007), *Nutraceuticals: A Guide for Healthcare Professionals*, 2nd Edition; Pharmaceutical Press London: ISBN: 9-78085369-659-9.
4. Murray, R.M., Harper, H.A., Harper, s. (2000), *Biochemistry*, 25th Edition; Appleton & Lange: ISBN: 9780838536841.
5. Robert, E.C., Wildman, Wildman, R., Wallace, T.C. (2016), *Handbook of Nutraceuticals and Functional Foods*. 2nd Edition; CRC Press: ISBN: 9781420006186.
6. Voet, D., Voet, J.D. (2011), *Biochemistry*, 4th Edition; John-Wiley & Sons: Canada, ISBN: 9780470917459.

Structure Elucidation of Inorganic Materials

Course Code: CHM-760

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objectives of this course are

- To demonstrate about the synthesis, characterization and applications of modern inorganic materials.
- It enables students for the development of new functional materials in areas such as energy, catalysis and electronic materials. **Learning Outcomes**
 - Demonstrate about the synthesis, characterization and applications of modern inorganic materials.
 - Enable students for the development of new functional materials in areas such as energy, catalysis and electronic materials.

Course Outline

Unit 1. Methods

Solid State Reaction or Shake'n Bake Methods. Low Temperature or Chimie Douce Methods. Gas-Phase Methods. High-Pressure Methods.

Unit 2. Crystal Growth

Crystal Growth. Identification of Crystalline Solids. Structure of Non-Molecular Crystalline Solids. Defects. Impurities and Stoichiometry of Crystalline Solids.

Unit 3. Diffraction Studies

X-Ray Diffraction. Electron Diffraction. Neutron Diffraction Microscopy.

Unit 4. Spectroscopy

Optical and Electron Microscopy Techniques. Vibrational, Visible and Ultraviolet (UV) spectroscopy. Nuclear Magnetic Resonance (NMR) spectroscopy. Electron Spin Resonance (ESR) spectroscopy. Electron spectroscopy. Mossbauer spectroscopy.

Unit 5. Thermal Analysis

Thermal Analysis Thermogravimetry (TG). Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC). Strategy to Identify, Analyze and Characterize Unknown solids.

Recommended books/reference material

1. Brisdon, A. K. (1998). *Inorganic Spectroscopic Methods*. (1st ed.). Oxford University Press.
2. Brisdon, N. K. (2010). *Inorganic Spectroscopic Methods*. Oxford University Press, United Kingdom.
3. Lalena, J. N., Cleary, D. A., Carpenter, E. E., & Dean, N. F. (2008). *Inorganic Materials Synthesis and Fabrication*, John Wiley & Sons, Inc., Hoboken, New Jersey.
4. Schubert, U. (2019). *Synthesis of Inorganic Materials*. (4th ed.). Wiley VCH Verlag GmbH & Co. KGaA, Germany.
5. Schubert, U. L., & Husing, N. (2000). *Synthesis of Inorganic Materials*. (1st ed.). Wiley-VCH Verlag GmbH & Co. KGaA, Germany.
6. Weller, M. T. (1995). *Inorganic Material Chemistry*. Oxford University Press, Inc., New York.
7. West, A. R. (2022). *Solid State Chemistry and its Applications*. (2nd ed.). John-Wiley & Sons, UK.
8. Williamson, E. M., & Brutchey, R. L. (2023). Using Data-Driven Learning to Predict and Control the Outcomes of Inorganic Materials Synthesis. *Inorganic Chemistry*, 62(40), 1625116262.

Green Chemistry

Course Code: CHM-761

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students should be able to understand the concepts of green chemistry and learn sustainability as the course contents relates to green chemistry.

- They will be able to understand the basic principles of green chemistry and differentiate between different types of solvents and learn how greener solvents are best alternate sources for various synthesis protocols?
- They will develop an understanding of alternate synthesis routes for various industrial products and develop a skill for energy efficient framework design.

Learning Outcomes

- Students will have deep understanding of green chemistry and sustainability. They will learn how greener solvents are best alternate sources.
- They will have command on using alternate synthesis routes for various industrial products and develop a skill for energy efficient framework design.

Course Outline

Unit 1. Introduction to Green Chemistry

Definition and concept, historical perspective and evolution of green chemistry. Global movements for sustainable development. (step towards green chemistry). Sustainable development goals and green chemistry, roots of innovation and 12 principles of green chemistry.

Unit 2. Tools of Green Chemistry

Renewable feedstock and biocatalysis, eco-friendly reagents. Green solvents, their properties and applications. Alternative products /Target molecules. Process analytical chemistry and alternative catalysts. Focus on the applications of innovative technology.

The development of. “greener” routes to improve industrial processes and to produce important products. Alternative synthetic routes (e.g. C-H bond activation).

Unit 3. Energy Efficiency & Emerging Technologies

Design for energy efficiency photochemical reactions processes. Advantages of and challenges faced by photochemical examples of photochemical reactions. Chemistry using microwaves. Microwave heating. Microwave assisted reactions. Sonochemistry and green chemistry examples of electrochemical synthesis.

Unit 4. Hydrogen Fuel Basics

The clean pollution free fuel. Hydrogen fuel from water. Fossil fuel. CH₄ and CH₃OH.

Hydrogen fuel cell technology. Mechanism of electricity generation in a fuel cell.

Unit 5. Renewable Resources and Green Chemistry Using Bio Catalytic Reactions

Solar Energy. Solar Photovoltaic System (PV cells). Solar thermal devices (STD). Wind energy. Geothermal energy. Hydrothermal energy. Oceanic power. Biomass energy. Biogas. Bio-fuel. Bio-diesel. Introduction to green chemistry using bio catalytic reactions. Fermentation and bio transformations. Production of bulk and fine chemicals by microbial fermentation. Bulk & fine Chemicals, antibiotics. Vitamins. Bio catalysis synthesis of industrial chemicals by bacterial constructs. Examples of green bio catalytic processes.

Recommended books/reference material

1. Ahluwalia, V.K. (2013). *Green Chemistry: A Textbook*. (1st ed.). Alpha Science International.
2. Ameta, S. C., & Ameta, R. (2023). *Green Chemistry: Fundamentals and Applications*. (2nd ed.). CRC Press, United States.
3. Gonzalez, J., & David, J. C. (2011). *Green Chemistry and Engineering: A Practical Design Approach*. (1st ed.). John Wiley and Sons.
4. Jing, H. H., Bardakci, F., Akgöl, S., Kusat, K., Adnan, M., Alam, M. J. & Sasidharan, S. (2023). Green carbon dots: Synthesis, characterization, properties and biomedical applications. *Journal of Functional Biomaterials*, 14(1), 27.
5. Kim, Y., & Li, C. J. (2020). *Green Synthesis and Catalysis*. (Vol. 1). Elsevier.
6. Torok, B., & Dransfield, T. (2017). *Green Chemistry: An Inclusive Approach*. (1st ed.). Elsevier.

Nanochemistry and Nanotechnology

Course Code: CHM-762

Credit Hours: 03

Pre-requisite: Nil

Objectives

- The objectives of this course are to impart the knowledge about the applications of nanochemistry for the synthesis of nano metal oxides.
- Guide about the significance of these oxides in advanced application.

Learning Outcomes

- Students will have deep understanding of key introductory concepts of nanochemistry and synthesis methods of nano metal oxides.
- They will have command on use of these nano metal oxides in various applications on commercial and industrial scale.

Course Outline

Unit 1. Synthesis of Nanomaterials Chemical Processes

Chemical precipitation and co-precipitation, polyol, and borohydrate reduction methods, Sol-Gel synthesis; Microemulsions synthesis, Hydrothermal, Solvothermal synthesis methods, Microwave assisted synthesis; Nonchemical assisted synthesis, Core-Shell nanostructure, Organic-Inorganic hybrid Nano composites, Porous materials, Quantum dot (QDs) synthesis, self-assembly of nanostructures.

Unit 2. Types of Nanomaterials

Nano-metal oxides, Graphene based materials, Green synthesized materials, 2D and 3D nanomaterials, textural characterization techniques, applications.

Unit 3. Physical Properties of Nanomaterials

Size effect of Nanomaterials: Size, shape, density, melting point, wettability and specific surface area. Electronic properties: Electronic conductivity, band gap tuning - band gap determination – Piezoelectric and ferroelectric materials and their behaviour and applications. Magnetic properties: Magnetic hysteresis, superparamagnetism- Optical properties: Electroluminescence, Photoluminescence, Jablonski diagram, fluorescence and phosphorescence, Optical properties of nanostructures.

Unit 4. Characterization of Nanomaterials

Different characterization techniques such as Fourier Transform Infrared (FTIR), Nuclear Magnetic Resonance (NMR), UV-VIS, Raman, Scanning Electron Microscopy (SEM).

Transmission Electron Microscopy (TEM), Thermogravimetric analysis (TGA), Differential Scanning Calorimeter (DSC), X-ray Diffraction (XRD), Energy Dispersive Spectroscopy (EDS), X-ray Phosphorescence Spectroscopy (XPS) etc.

Unit 5. Applications

Advanced applications of nano-materials in Air, Water, soil, Agriculture, Food. Nanomaterials for Photovoltaic Solar Energy Conversion Systems, Nanomaterials for Energy Storage Systems etc.

Recommended books/reference material

1. Brechignac, C., Houdy, P., & Lahmani, M. (2006). *Nanomaterials and Nanochemistry*, Springer-Verlag.
2. Fierro, J. L. G., (2006). *Metal Oxides Chemistry and Applications*, Taylor & Francis.
3. Niederberger, M., & Pinna, N. (2009). *Assembly and Application*, Springer.
4. Raneesh, B., Visakh, P. M. (2020). *Metal Oxide Nanocomposites: Synthesis and Applications*, LLC. ISBN:9781119363576
5. Rayees, A. Z. (2023). *Metal Oxide Nanocomposite Thin Films for Optoelectronic Device Applications*, LLC. ISBN: 978-1-119-86508-7
6. Sharma, A., & Oza, G. (Eds.). (2023). *Nanochemistry: Synthesis, Characterization and Applications*. CRC Press
7. Velammal, M. (2023). *Nano Chemistry-Overview. Frontiers in Chemical, Biological and Pharmaceutical Science*.
8. Visakh, P. M., & Maria, J. M. M. (2016). *Nanomaterials and Nanocomposites: Zero-to Three-Dimensional Materials and Their Composites*, Wiley-VCH Verlag GmbH & Co. KGaA.

Physical Aspect of Polymers Course

Code: CHM-763

Credit Hours: 03

Pre-requisite: Nil

Objectives

The objective of this course is to study physical aspects of the polymers and Polymer thermodynamic properties.

Learning Outcomes

- Students will have understanding of polymer solutions, their measurement techniques and properties.
- They will have command on surface structural nature and various applications of polymers.

Course Outline

Unit 1. Conducting Polymers and Molecular Weight Determination

Synthesis of aromatic polyethers, polyacetals, polyamides, polyurethane, polymers with metal in their backbone, P and S containing polymers, Biopolymers, Biodegradable polymers, Fire retardant polymers, Liquid crystalline polymers - Molecular weight of polymers: Number average, weight average and viscosity average molecular weights of polymers - Determination of molecular weight of polymers by GPC and Viscometry methods - Thermal analysis of polymers using DSC, TGA, DTA, and DMA. Conducting Polymers: Discovery – Conducting mechanism – Classification of conducting polymers: Intrinsic and extrinsic conducting polymers - Chemical and electrochemical methods for the synthesis of conducting polymers – Applications of conducting polymers in corrosion protection, electrochemical energy devices and sensors.

Unit 2. Polymer Surfaces and Interfaces

Thermodynamics of surfaces and interfaces, crystalline and glassy polymers, theoretical polymer blend interphase thickness, determination of interior surface areas, conformation of polymer chains in a polymer blend interphase.

Unit 3. Physical Parameters

Physical parameters affecting the chain dimensions, Theta conditions, Polymer Kinetics, Thermodynamic studies of polymers.

Unit 4. Structure and Nature of Polymers

Amorphous and crystalline structures, Semicrystalline nature, viscoelasticity models and predictions, time-temperature dependency, polymer rheology.

Unit 5. Properties and Applications of Polymers

Electrical, magnetic, chemical and optical properties of polymers. Application in various fields of Physical Sciences.

Recommended books/reference material

6. Ahluwalia, V, K, & Mishra, A. (2008). *Polymer science: a textbook*. (1st ed.). CRC Press. ISBN: 978-1420068191
7. Bhatnagar, M. S. & Misra, C. K. (2004). *Textbook of polymers*. Chand (S.) & Co Ltd ,India. ISBN: 978-8121923460
8. Carraher Jr, C. E. (2013). *Seymour/Carraher's polymer chemistry*.(9th ed.). CRC Press. ISBN: 978-1466552036
9. Carraher Jr, C. E. (2017). *Introduction to polymer chemistry*. (4th ed.). CRC Press. ISBN: 9781498737616
10. Chyr, G., & DeSimone, J. M. (2023). *Review of high-performance sustainable polymers in additive manufacturing*. *Green Chemistry*, 25(2), 453-466.
11. Fried, J. R. (2014). *Polymer science and technology*. (3rd ed.). Prentice Hall. ISBN: 9780137039555
12. Furnkaw, J. (2003). *Physical chemistry of polymer rheology*, Springer. ISBN: 9783540000532
13. George, O. (2004) *Principles of polymerization*. (4th ed.). Wiley India. ISBN: 9788126513918
14. Hiemenz, P. C., & Lodge, T. P. (2007). *Polymer chemistry*. (2nd ed.). CRC Press. ISBN: 9781574447798
15. Li, L., Han, L., Hu, H., & Zhang, R. (2023). *A review on polymers and their composites for flexible electronics*. *Materials Advances*, 4(3), 726-746.
16. Patterson, G. (2007). *Physical chemistry of macromolecules*.(1st ed.). CRC Press. ISBN: 9780824794675
17. Ravve, A. (2012). *Principles of polymer chemistry* (3rd ed.). Springer. ISBN: 9781461422112
18. Sundararajan, P. R. (2016). *Physical Aspects of Polymer Self-Assembly*. Wiley India. ISBN: 978-1-118-99439-9

Research Methodology and Statistical Analysis

Course Code: CHM-764

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students will acquire knowledge about the conduction of a literature survey and identification of research problems. Students will comprehend, how to handle data and

calculate various statistical parameters which may make the data meaningful. Students will learn about how to comprehend error, its types and distribution.

Learning Outcomes

- Concept of Research and Research Methodology: Modern tools for research, use of digital resources for literature survey and designing research problems, research ethics.
- Concept of error, its types: Distribution and propagation of error, theory and applications of statistical methods for the determination and elimination of errors in data.
- Use of spreadsheets for statistical analysis: Outliers, regression analysis and correlation constants.

Course Outline

Unit 1. Research Ethics

Introduction to research ethics: Definition and Importance, Ethical principles in chemical research: respect for persons, beneficence, and justice, Animal welfare and ethical treatment in research, Integrity in research: data fabrication, Falsification, and plagiarism, Conflict of Interest and disclosure policies, Ethical issues in publication and authorship, Intellectual property rights and patenting in chemical research, Ethical considerations in collaborative and interdisciplinary research, Ethical oversight and institutional review board.

Unit 2. Research Methodology

Conception of Research and Research Methodology: Modern ways for research, use of digital resources for literature survey, Formulating research questions and objectives, designing research problems, writing a research proposal: Structure, Content, and Formatting, research ethics.

Unit 3. Errors in Research

Concept of error, its types like Measurement Errors, sampling errors, systematic errors, random errors: Distribution and propagation of error, theory and applications of statistical methods for the determination and elimination of errors in data.

Unit 4. Statistical Analysis

Use of spreadsheets for statistical analysis: Outliers, regression analysis and correlation constants.

Unit 5. Articles, Project and Thesis Write Up

Understanding about writing skills of research for the purpose of thesis, projects and articles writing. Articles publication in Journals.

Recommended books/reference material

1. Research Methodology Methods and Techniques, 4th Ed., Kothari C.R., Guarav G, John Wiley & Sons, Inc., 2019.
2. Research Methodology, 2nd Ed., Panneerselvam R, Brooks/Cole-Cengage learning, Belmont CA, 2021.
3. Research Methodology, Concepts and Cases, 2nd Ed., Deepak C.,Neeha S, Freeman and Company, New York, USA, 2018.

Advanced Organic Synthesis

Course Code: CHM-765

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Students will familiarize with advanced synthetic methods beyond basic organic reactions, including multistep synthesis, organometallic reactions, and asymmetric synthesis and in addition they will have advanced mechanistic chemistry and applications of advanced radicals in organic synthesis

Learning Outcomes

- Students should be able to demonstrate proficiency in utilizing advanced synthetic methods, including multistep synthesis, transition metal-catalyzed reactions, and asymmetric synthesis, to construct complex organic molecules.
- They will have a deep understanding of reaction mechanisms involved in advanced organic reactions, enabling them to predict and rationalize reaction outcomes and propose mechanistic pathways for novel reactions.
- They will be able to design and plan synthetic routes for the efficient synthesis of target molecules, considering factors such as selectivity, yield, scalability, and sustainability.

Course Outlines

Unit 1. Asymmetric Synthesis Techniques

Introduction to Asymmetric Synthesis, Chiral Induction and Chirality, Enantioselective Catalysis (metal complexes, organocatalysts, and biocatalysts, Mechanistic aspects of enantioselective catalysis and stereoinduction, Applications of asymmetric catalysis in the synthesis of complex molecules), Asymmetric Transformations (Strategies for achieving stereochemical control in

asymmetric synthesis: kinetic resolution, dynamic kinetic resolution, and desymmetrization), Importance of chirality and enantiomeric purity in pharmaceuticals, agrochemicals, and materials science.

Unit 2. Organometallics in Organic Synthesis

Organometallic Reaction Mechanisms, Catalytic C-C Bond Formation including crosscoupling reactions (e.g., Suzuki-Miyaura, Heck, and Negishi reactions), transition metalcatalyzed asymmetric hydrogenation reactions Pd-catalysed coupling reactions.

Unit 3.

Selective Aldol Reactions

Classical Aldol Condensation (reaction involving enolates and carbonyl compounds, intra- and intermolecular aldol reactions Stereochemistry of aldol condensation products and factors influencing stereoselectivity), Regioselectivity and Chemoselectivity (Factors affecting regioselectivity in aldol reactions: steric hindrance, electronic effects, and substrate reactivity, Chemoselective aldol reactions: strategies for controlling the selectivity of multiple carbonyl groups). Catalytic Aldol Reactions Asymmetric Aldol Reactions including chiral auxiliary methods, chiral ligands, and asymmetric organocatalysis.

Unit 4. Alkenes Synthesis

Traditional Methods of Alkene Synthesis including elimination reactions, addition reactions to alkenes, and reduction of alkynes and carbonyl compounds, Transition MetalCatalyzed Cross-Coupling Reactions, Alkene Synthesis via Olefination Reactions including Wittig, Horner-Wadsworth-

Emmons (HWE), Julia-Kocienski, and Tebbe reactions, Hydrofunctionalization Reactions including hydroboration, hydroamination, hydroxylation, and hydroacylation for the selective synthesis of alkenes.

Unit 5. Cyclisation Reactions

Intramolecular cyclization reactions involving the formation of cyclic compounds from linear precursors. Types of intramolecular cyclization reactions including ring-closing reactions and cascade reactions. Intermolecular Cyclization Reactions that involve coupling of two or more molecules to form cyclic products such as Diels-Alder reactions and FriedelCrafts reactions.

Unit 6. Protecting Group Chemistry

Introduction to Protecting Groups (Definition and importance of protecting groups in organic synthesis), Overview of functional groups prone to undesired reactions during synthetic transformations, Basic principles underlying protection and deprotection reactions, Factors influencing the choice of protecting groups, including stability, selectivity, and ease of introduction and removal. Common Protecting Groups and Protecting Group Strategies (Strategies for selective protection and deprotection of multiple functional groups in complex molecules, Planning and implementation of protection and deprotection sequences in organic synthesis, Compatibility of protecting group manipulations with other reaction conditions and functional groups).

Recommended Books/reference material

1. Clayden, J., Greeves, N., & Warren, S. (2020). *Organic Chemistry* (3rd ed.). Oxford: Oxford University Press, ISBN: 9780199270293.
2. Francis A., & Richard J. S. (2007). *Advanced Organic Chemistry Part A* (5th ed.). Lower Manhattan, New York City: Spring Street, ISBN-13: 978-0-387-44897-8.
3. Francis, A., & Richard J. S. (2007). *Advanced Organic Chemistry Part B* (5th ed.). Lower Manhattan, New York City: Spring Street,, ISBN-13:978-0-387-68350-8.
4. Kurti L & Czako B. (2005). *Strategic Applications of Named Reactions in Organic Synthesis* (1st ed.). 84 Theobald's Road, London WC1X 8RR, UK: Elsevier Academic Press, ISBN: 9780080575414.
5. Smith, M. B. & March, J. (2013). *March's Advanced Organic Chemistry* (7th ed). Hoboken, New Jersey, USA: JohnWiley & Sons, ISBN: 978-0-470-46259-1.

Molecular Fluorescence

Course Code: CHM-766

Credit Hours: 03

Pre-requisite: Nil

Objectives

- To teach students the fundamental understanding of the principles underlying fluorescence spectroscopy, including excitation and emission processes, Jablonski diagram, Stokes shift, and fluorescence lifetime.
- To familiarize students with the properties and applications of fluorescent probes and labels used in various fields, including biology, chemistry, materials science, environmental science, and medical diagnostics, and quantitative and qualitative analysis.

Learning Outcomes

- Students should be able to use the technique in different fields like biology, chemistry, materials science, environmental science, and medical diagnostics.
- They will learn quantitative analysis techniques using fluorescence spectroscopy, including calibration methods, standard addition, internal standards, and multivariate analysis methods for complex datasets.

Course Outlines

Unit 1. Introduction to Molecular Fluorescence

Overview of fluorescence phenomenon, principles, and applications in various fields such as chemistry, biology, materials science, and medicine.

Unit 2. Fluorescent Molecules and Chromophores

Discussion of the electronic structure and properties of fluorescent molecules and chromophores. Concepts of excitation and emission wavelengths, Stokes shift, and quantum yield.

Unit 3. Fluorescence Spectroscopy Techniques

Introduction to fluorescence spectroscopy techniques including steady-state fluorescence spectroscopy, time-resolved fluorescence spectroscopy, fluorescence lifetime measurements, and fluorescence polarization.

Unit 4. Fluorescence Probes and Labels

Study of fluorescent probes and labels used for specific biomolecules and cellular structures in fluorescence microscopy, flow cytometry, and other imaging techniques.

Unit 5. Fluorescence Quenching and Enhancement

Mechanisms and factors influencing fluorescence quenching and enhancement including collisional quenching, Förster resonance energy transfer (FRET), and photoinduced electron transfer (PET).

Unit 6. Fluorescence Imaging Techniques

Overview of fluorescence imaging techniques such as confocal microscopy, multiphoton microscopy, fluorescence in situ hybridization (FISH), and fluorescence resonance energy transfer (FRET) microscopy, Live cell imaging and time-lapse imaging.

Unit 7. Applications of Molecular Fluorescence

Exploration of applications of molecular fluorescence in various fields including analytical chemistry, biochemistry, environmental monitoring, drug discovery, and medical diagnostics, materials science including fluorescent polymers, nanoparticles, quantum dots, and molecular sensors, Study of fluorescence in biological systems including protein folding studies, enzyme kinetics, ligandreceptor interactions, and intracellular signaling pathways.

Recommended Books//reference material

1. Alexander P. Demchenko, (2010) *Advanced Fluorescence Reporters in Chemistry and Biology II : Molecular Constructions, Polymers and Nanoparticles*, SpringerVerlag Berlin and Heidelberg GmbH & Co. KG, Berlin, Germany, ISBN:13 9783642046995
2. Bernard V., Mário N. & Berberan S. (2012). *Molecular Fluorescence: Principles and Applications*, (2nd Edition) John Wiley & Sons, Inc. ISBN: 978-3-527-328376
3. Bernard. V. & Jean C. B. (2012). *New Trends in Fluorescence Spectroscopy: Applications to Chemical and Life Sciences* (1st ed. Springer-Verlag Berlin and Heidelberg GmbH & Co. KG, Berlin, Germany. ISBN:13-9783642632143
4. Joseph R. & Lakowicz, (2006). *Principles of Fluorescence Spectroscopy* (3rd edition). Springer-Verlag US ISBN: 978-1-4899-7880-6
5. Markus S., Johan H. & Jörg E. (2011). *Handbook of Fluorescence Spectroscopy and Imaging: From Ensemble to Single Molecules*. ISBN: 978-3-527-31669-4
6. Valeur, B. (2001). *Molecular Fluorescence: Principles and Applications*. WileyVCH Verlag GmbH, Weinheim, Germany. ISBN: 3-527-60024-8.

Named Reactions in Organic Synthesis

Course Code: CHM-767

Credit Hours: 03

Pre-requisite: Nil

Objectives

- To teach students the graphically visualization of organic reactions with correct reaction mechanisms
- Visualize them the stereochemical (and eventual regiochemical) outcome for organic reactions Substitution, elimination, addition of electrophiles to alkenes and some additions of nucleophiles to a number of representative carbonyl compounds

Learning Outcomes

- Students should be able to identify and recognize key organic named reactions, understanding their reaction mechanisms, substrates, and products.
- They will be capable of designing and planning synthetic routes using organic named reactions, considering factors such as selectivity, yield, stereochemistry, and functional group compatibility.

Course Outlines

Unit 1. Oxidation and Reduction Reactions

Study of named reactions involving oxidation and reduction reactions, including the Jones oxidation, Swern oxidation, Clemmensen reduction, Wolff-Kishner reduction and their synthetic applications.

Unit 2.

C-C Bond Formation Reactions

Discussion of named reactions involving carbon-carbon bond formation reactions, including the Wittig reaction, Grignard reaction, and SuzukiMiyaura coupling, Aldol Condensation.

Unit 3.

Rearrangement Reactions

Claisen Rearrangement, Beckmann Rearrangement, Cope Rearrangement, Fries Rearrangement, Baeyer-Villiger Oxidation, Pinacol Rearrangement, Wagner-Meerwein Rearrangement, Stevens Rearrangement, Benzilic Acid Rearrangement, Wittig Rearrangement.

Unit 4.

Reactions Involving Metal Reagents

Suzuki-Miyaura Coupling, Heck Reaction, Sonogashira Coupling, Negishi Coupling, Stille Coupling, Buchwald-Hartwig Amination, Grignard Reaction.

Unit 5. Multicomponent Reactions

Ugi reaction, Passerini Reaction, Biginelli Reaction, Hantzsch Dihydropyridine Synthesis, Petasis Reaction, Bucherer-Bergs Reaction.

Recommended Books//reference material

1. Clayden, J., Greeves, N., & Warren, S. (2012). *Organic Chemistry* (2nd ed.). Oxford, UK: Oxford University Press: ISBN: 9780199270293.
2. Kurti, L., & Czako, B. (2005) *Strategic Applications of Name Reactions in Organic Synthesis*. Academic Press: New York, ISBN: 9780080575414.
3. Laue, T., & Plagens, A. (1998). *Name Organic Reactions*. New York, John Wiley and Sons: Chichester, ISBN: 0-471-97142-1.

4. Li, J. J. (2014). *Name Reactions: A Collection of Detailed Reaction Mechanisms* (5th ed.). Berlin: Springer-Verlag, ISBN: 978-3-319-03979-4
5. Mundy, B. P., & Ellerd, M. G. (2005). *Name Reactions and Reagents in Organic Synthesis*. New York: John Wiley, ISBN: 9780471228547.

Modern Heterocyclic Chemistry

Course Code: CHM-768

Credit Hours: 03

Pre-requisite: Nil

Objectives

This course aims to provide the students a fundamental theoretical understanding of heterocyclic chemistry. The students will explore the intricacies of these compounds, including their structural properties, reactivity, and applications.

Learning Outcomes

- Student will have knowledge about the synthesis of heterocyclic systems and their applications in drug development.
- This knowledge will also empower them to design synthetic routes for practically significant heterocyclic compounds.

Course Outlines

Unit 1. Classification and Significance Of Heterocyclic Compounds

Classification and nomenclature of heterocyclic compounds.

Understanding the significance of heterocycles in various fields.

Unit 2. Structures and Spectroscopic Properties

Structural properties of aromatic heterocycles. Some spectroscopic properties of heteroaromatic systems, (Ultraviolet/Visible (Electronic) Spectroscopy, Nuclear Magnetic Resonance (NMR) Spectroscopy).

Unit 3. Ring Synthesis of Aromatic Heterocycles

Six-membered ring synthesis, five-membered ring synthesis, threemembered ring synthesis, synthesis of fused ring systems, heterocycles containing a ring-junction nitrogen (bridgehead compounds), heterocycles containing more than two heteroatoms, saturated and partially unsaturated heterocyclic compounds: reactions and synthesis.

Unit 4. Reactions Involving Heterocycles

ANRORC (Addition of the nucleophile, ring opening, and ring closure) and various nucleophilic substitutions in heterocycles, modern synthetic cyclization methods like neutral, cationic and anionic cyclization, cycloaddition reactions with multicomponent systems.

Unit 5. Heterocycles in Biochemistry: Heterocyclic Natural Products

Heterocyclic amino acids, enzyme co-factors; heterocyclic vitamins; Coenzymes, ribonucleic acid (RNA) and deoxyribonucleic acid (DNA); genetic information; purines and pyrimidines, heterocyclic natural products. Alkaloids, marine heterocycles, halogenated heterocycles, macrocycles containing oxazoles and thiazoles, other nitrogencontaining natural products including anthocyanins and flavones

Unit 6. Applications in Drug Discovery and Medicinal Chemistry

Role of heterocyclic compounds in drug design and development, Structureactivity relationship (SAR) studies of heterocyclic drugs, examples of clinically important heterocyclic drugs.

Unit 7. Role of Heterocycles as Materials in Catalysis

Heterocyclic polymers and materials, Heterocyclic compounds use as catalysts and catalyst supports, Applications of heterocyclic chemistry in green and sustainable chemistry.

Recommended Books/reference material

1. Clayden, J., Greeves, N., & Warren, S. (2000). *Organic Chemistry* (2nd ed.). Great Clarendon Street, Oxford OX2 6DP: Oxford University Press, ISBN: 9780-19927-029-3.
2. Joule, J.A., & Keith, M. (2010). *Heterocyclic Chemistry* (5th ed.). The University of Manchester, UK Keith Mills: Wiley-Blackwell, ISBN: 978-1-40513300-5.
3. Katritzky, A. R. (2019). *Advances in Heterocyclic Chemistry*. University of Florida, Gainesville, USA, ISBN: 9780128001714.
4. Scriven, E.F.V., & Ramsden, C.A. (2016). *Advances in Heterocyclic Chemistry* (vol. 118). Portland, Oregon, USA: Wiley Interscience, ISBN: 978-0-12804696-8.

5. Van der Eycken, E. V., & Sharma, U. K. (2022). *Multicomponent reactions towards heterocycles*. Weinheim: Wiley.
6. Vaquero, J. J. Barluenga, J. (2011). *Modern Heterocyclic Chemistry* (1st ed.). Boschstr. 12, 69469 Weinheim, Germany: John-Wiley and Sons, ISBN: 978-3527-33201-4

Chirality in Coordination Chemistry

Course Code: CHM-769

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Students will acquire knowledge about the key introductory concepts of Chiral Organometallic Complexes as well as using this knowledge for qualitative and quantitative analysis of chiral compounds.
- To familiarize the students with historical background of coordination compounds and will be able to predict shape of a complex based on spin only magnetic moment.

Learning Outcomes

- Students will have deep understanding about the research in the areas of chiral inorganic, supramolecular coordination compounds and complex materials.
- Student will be able to describe and explain the bonding in coordination compounds using Effective Atomic Number Rule (18-electron rule), Valence Bond Theory, Crystal Field Theory and Molecular Orbital Theory; compare the bonding theories.

Course Outline

Unit 1. Fundamental Concepts of Coordination Chemistry and Chirality

Definition and Recognition of Coordination Compounds (Complexes), Werner's Contributions to Coordination Chemistry, Electrolyte and Non-Electrolyte Complexes, Ligands, Application and Importance of Coordination Compounds, Introduction to chirality and its significance in coordination chemistry.

Unit 2. Chiral Ligands and Complexes

Design and synthesis of chiral ligands for coordination chemistry, Coordination modes and stereochemistry of chiral ligands, Properties and characterization of chiral coordination complexes.

Unit 3. Chirality Transfer in Coordination Complexes

Mechanisms of chirality transfer from chiral ligands to metal centers, Influence of coordination geometry and ligand environment on chirality transfer, Stereoselective synthesis and resolution of chiral coordination complexes, Chiral recognition phenomena in coordination chemistry, Host-guest interactions and molecular recognition in chiral coordination complexes, Applications of chiral recognition in catalysis, sensing, and separation.

Unit 4. Asymmetric Catalysis

Chiral catalysts and asymmetric catalytic transformations in coordination chemistry, Asymmetric induction and enantioselectivity in metal-catalyzed reactions, Mechanistic insights into asymmetric catalysis.

Unit 5. Preparation and Reactions of Coordination Complexes

Methods for preparation of coordination complexes, Ligand substitution reactions: associative and dissociative mechanisms, Redox reactions and electron transfer processes in coordination chemistry, Acid-base reactions and protonation of coordinated ligands.

Mechanistic aspects of substitution reactions: inner sphere and outer sphere mechanisms.

Factors influencing reaction rates: steric hindrance, electronic effects, and solvent effects, Homogeneous and heterogeneous catalysis by coordination complexes, Catalytic cycles and intermediates in organometallic catalysis, Applications of coordination complexes as catalysts in organic transformations.

Unit 6. Chirality in Supramolecular Chemistry

Supramolecular assemblies and chiral architectures in coordination complexes, Chiral selfassembly and hierarchical organization of coordination compounds, Applications of chiral supramolecular structures in materials science and nanotechnology.

Unit 7. Chirality in Coordination Polymers and Metal-Organic Frameworks (MOFs)

Design and synthesis of chiral coordination polymers and MOFs, Applications of chiral MOFs in gas storage, separation, and catalysis, Chiral-induced spin selectivity in coordination polymers.

Unit 8. Physical Methods of Structural Investigation

Methods used in Structural Investigation of Complexes: Electronic Spectroscopy, Vibrational Spectroscopy, Magnetic Measurement, Circular dichroism (CD), optical rotation (OR), and vibrational circular dichroism (VCD), X-ray crystallography.

Recommended books/reference material

1. Amouri, H., & Gruselle, M. (2008). *Chirality in Transition Metal Chemistry: Molecules, Supramolecular Assemblies and Materials*. John Wiley & Sons, Ltd.
2. Geoffrey, A. L. (2010). *Introduction to Coordination Chemistry*. John Wiley and Sons, Ltd.
3. Gispert, J. R. (2008). *Coordination Chemistry*. Wiley-VCH Verlag GmbH & Co. KGaA.
4. Morales, D. M. (2018). *Pincer Compounds: Chemistry and Applications* (1st ed.). Elsevier Inc.
5. Schulte, T. R. (2019). *Metal- and Ligand-centered Chirality in Square-planar Coordination Compounds*. Georg-August-Universität Göttingen.
6. Soni, P.L. Soni, V. (2021). *The Chemistry of Coordination Complexes and Transition Metals*. Taylor & Francis.

Literature Review and Seminar Course

Code: CHM-776

Credit Hours: 03

Pre-requisite: Nil

Objectives

- To learn review and assess scientific literature critically.
- To write and present an overview of the relevant literature for a specific research topic.
- To identify important unanswered questions in the field.
- To help the doctoral students to write the research article and research proposals.

Learning Outcomes

- Students will have deep understanding about the literature review and will be able to Identify and select relevant sources for a literature review.
- Student will be able to critically analyze and evaluate existing literature in a specific field.

Course Outline

- Unit 1. Introduction to Literature Review**
Overview of the importance of literature reviews in research, Understanding the components of a literature review, Identifying sources and literature search strategies.
- Unit 2. Research Methodologies**
Introduction to various research methodologies, choosing the appropriate methodology for a literature review, Ethical considerations in literature review research. Writing Research Article, Project understanding. Selection of topic. Experimental design. Formulate an idea. Make an outline. Writing research article include topic, authors names and affiliation, abstract, keywords, introduction, materials and methods, results and discussion, author contribution, acknowledgements, references, highlights and graphical abstract. Examples.
- Unit 3. Critical Analysis of Literature**
Developing skills in critically analyzing research papers, Synthesizing information from diverse sources, Identifying gaps and controversies in existing literature
- Unit 4. Writing Review Article**
Types of review article including narrative, systematic, scoping and mini reviews. Elements of review article including title, authors names and affiliation, abstract, table of contents, introduction, main body, conclusion, acknowledgements, references and concept map. Examples.
- Unit 5. Seminar Presentations and Peer Review**
Understanding the structure of a seminar presentation, creating effective presentation slides, Rehearsing and refining oral communication skills, Students present their literature reviews in a seminar format, Peer feedback and constructive criticism. Reflection on the seminar experience and improvement strategies.

Recommended books/reference materials

1. Booth, A. Sutton, A. Clowes, M. James, M. M-St. (2021). *Systematic Approaches to Association*.
2. Diana, R. (2012). *The Literature Review: A Step-by-Step Guide for Students*. SAGE
3. Mahrool, F. (2020). *Research Methodology. A Guide for a Literature Review*. GRIN Publications.
4. Sarma, M. (2010). *Research methodology: Assignment, Seminar Paper & Project*. Eastern Successful Literature Review. SAGE Publications Book House.

5. Susanne, H. (2020). *Conducting Your Literature Review*. American Psychological Verlag.

Drug Designing and Drug Development Course

Code: CHM-777

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students will acquire understanding about the steps involved in drug designing and drug development. They will learn about applications of different softwares used in computer aided drug designing and drug development. They will also acquire knowledge about drug stability and prodrugs applications in drug designing.

Learning Outcomes

- Students will gain understanding about designing research projects in drug designing.
- Students will be able to know about intellectual property rights and patent fillings.
- Students will be able to learn about pharmaceutical industrial testing of stability of drugs.

Course Outline

Unit 1. Introduction to Drug Design and Drug Development

Terms used. Brief discussion of research phases of drug discovery. Target identification, lead identification, lead optimization, preclinical, clinical phases and approval phase. ADME and PK Properties. Bioavailability.

Unit 2. Molecular Modeling and Drug Development

Terms used. In-silico drug designing. Structure based drug designing. Ligand based drug designing. Role of different softwares in computer aided drug designing.

Unit 3.

Application of Prodrugs in Drug Development

Concept of prodrugs. Promoiety. Types of prodrugs. Discovery of sulfonamides. Applications of prodrugs in dosage forms. Examples of prodrugs of NSAIDs, antibiotics and anticancer drugs. Role of drug metabolism in increasing or decreasing duration of action.

Unit 4.

Drug Stability Studies

Factors affecting stability of drugs. Stability testing in pharmaceutical industries. Types of stability testing. GMP requirements regarding stability, FDA guidelines and stability protocols. Introduction to product stability of different pharmaceutical dosage form (tablets, capsule, suspensions, solutions, emulsions, ointments).

Unit 5.

Industrial Considerations

Intellectual property. The value of new ideas. Patents. Academic or government agreements. Leaner, meaner startups. Big company small company collaborations. Combination therapeutics.

Recommended Books/reference material

1. Powl, K.L. (2012) *A Textbook of Drug Design and Development*. Second Edition. Harwood Academic Publishers.
2. David, A.W. Foye, W.O. (2013). *Foye's Principles of Medicinal Chemistry*. 7th Edition, Verghese Publishing House.
3. John M.B. (2004). *Organic Medicinal and Pharmaceutical Chemistry*. 11th Edition. Edited by John H. Block. Lippincott Williams & Wilkins.
4. Richard, B.S. (2004). *The Organic Chemistry of Drug Design and Drug Action*. Edited by Academic Press. An Imprint of Elsevier.
5. Burger, A. (2021) *Medicinal Chemistry*. John Wiley & Sons. New York.
6. Robert M.R. (2022). *Real World Drug Discovery A Chemist Guide to Biotech and Pharmaceutical Research*. Elsevier, Kidlington, Oxford, UK, 2022.

Advanced Analytical Chemistry Techniques

Course Code: CHM-778

Credit Hours: 03

Pre-requisite: Nil

Objectives

Students will acquire knowledge about to

- Establish concise overview of the principles and practice of analytical methodology and data handling.
- Provide a useful resource for practicing analysts, seeking a summary of the principles of techniques and methods.

Learning Outcomes

- Students will have understanding of different advanced analytical techniques
- They will have command and operational skill on various analytical techniques

Course Outline

Unit 1. Sample Preparation for Metal Analysis

Different Methods for Preparation of samples for metals analysis.
Contamination during Metal Analysis. Safe Handling of Acids.

Unit 2. Sample Preparation for Microscopic and Spectroscopic Characterization

Sample preparation for microscopic and spectroscopic characterization of solid surfaces and films. Thermal Etching, Specimen Thinning for TEM.

Unit 3. Reactive Ion Techniques

Chemical Polishing and electro polishing. Ultramicrotomy. Surface enhancement by sample preparation techniques in Raman and Infrared spectroscopy.

Unit 4. Raman Spectroscopy and Other Techniques

Surface-Enhanced Raman Spectroscopy. Electrochemical Techniques. Vapor Deposition and Chemical Preparation Techniques. Colloidal Sol Techniques. Nanoparticle Arrays and Gratings.

Unit 5. Applications

Applications of analytical techniques in different disciplines of chemistry.

Recommended books/reference material

1. Fifiield F. W. & David K. (2000). *Principles and Practice of Analytical Chemistry*, 5th Edition, John Wiley & Sons, Inc., Hoboken, New Jersey. ISBN: 9780-632-05384-1.

2. Jaroslava S. G. (2011). *Sampling and Sample Preparation in Analytical Chemistry (Chemistry Research and Applications: Chemical Engineering Methods and Technology)* Nova Science Pub Inc. ISBN: 13-978-1621002697.
3. Mitra, S. (2003). *Sample Preparation Techniques in Analytical Chemistry*. John Wiley & Sons, Inc., Hoboken, New Jersey. ISBN: 0-471-32845-6.
4. Markus S., (1997). *Sampling and Sample Preparation Practical Guide for Analytical Chemists* Springer-Verlag Berlin Heidelberg. ISBN: 978-3-642-644863.
5. Zoltan M. & Ralph S. (2003). *Sample Preparation for Trace Element Analysis*, 1st Edition Volume 41 Elsevier Science ISBN: 9780444511010.

Advanced NMR Spectroscopy

Course Code: CHM-779

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Have advanced and instrumental aspects of NMR spectroscopic techniques.
- Develop ability to rationally wide variety of materials for characterization in academic research or industrial research.

Learning Outcomes

- Students will learn about advanced NMR spectroscopy, ^1H and ^{13}C chemical shift and coupling constant.
- They will have command on different NMR techniques like 1-D NMR, 2-D-NMR, DEPT, NOE, COSY, HECTOR, HMBC, INADEQUATE and NOESY.

Course Outline

Unit 1. Advanced Techniques in One-Dimensional NMR Spectroscopy

Overview of One-Dimensional NMR Spectroscopy' ^1H NMR and ^{13}C NMR shifts. Chemical shifts in ^{13}C NMR. Principles of Fourier Transform NMR, Selective Excitation and Decoupling Technique, Proton-coupled and decoupled

^{13}C NMR. Brief introduction to DEPT (The distortion less enhancement by polarization transfer), Quantitative NMR Spectroscopy.

Unit 2. Peak Broadening in NMR Spectroscopy

Introduction to peak broadening phenomenon in NMR spectroscopy and factors contributing to peak broadening; Intrinsic peak broadening mechanisms like homogeneous and inhomogeneous line broadening and natural line width and T2 relaxation; Extrinsic peak broadening effects like sample homogeneity and purity, Magnetic field inhomogeneity and instrumental artifacts; Strategies to minimize peak broadening; Effects of peak broadening on spectral resolution; Advanced techniques for deconvolution of broadened peaks like line shape fitting methods and fourier transform techniques; Exchangeable protons and solvent effects on chemical shift.

Unit 3. Decoupling and NOE Technique

Introduction to decoupling in NMR spectroscopy: Basic principles of SpinSpin Coupling, Role of decoupling in simplifying NMR spectra; Pulse sequences for decoupling: Continuous Wave (CW) Decoupling and pulse decoupling techniques (e.g., WALTZ, GARP); Applications of decoupling in NMR spectroscopy: Analysis of complex spectra and determination of scalar coupling constants, Basic principal and theory of NOE and its relation to molecular structures, Types of NOE experiment; NOESY (Nuclear Overhauser Effect Spectroscopy), ROESY (Rotating-frame overhauser Effect Spectroscopy), Techniques as a combination to determine the structure of an unknown organic molecule using some selected examples.

Unit 4. 2-D NMR Spectroscopy

Introduction and Basic principles 2-D NMR spectroscopy, of Advanced Pulse Sequences and Multi-Dimensional NMR Experiment, 2D-variations of NMR spectroscopy with special emphasis on COSY (correlation spectroscopy), Homonuclear COSY, Heteronuclear COSY. HSQC (Heteronuclear single quantum coherence spectroscopy). HECTOR (Heteronuclear correlation spectroscopy). HMBC (Heteronuclear multiple bond correlation). INADEQUATE (Incredible natural abundance double quantum transfer experiment). NOESY (Nuclear overhauser effect spectroscopy). Solid-state NMR spectroscopy.

Unit 5. Applications of NMR Spectroscopy

Structural elucidation of organic molecules, Stereochemistry analysis, Protein structure determination, Characterization of Protein-ligand interactions, Disease diagnosis and monitoring, Drug discovery and development and ligand screening and binding affinity studies, Lead Optimization and Structure-activity relationship (SAR) analysis, NMR in environmental monitoring like analysis of water and soil samples, Quality control and safety assessment.

Recommended books/reference material

1. Beauchamp, Phil. (2016). *Advanced Organic Spectroscopy Tools for Beginning Organic Spectroscopists: Using simulated spectra to learn how to solve complicated organic structures* (1st ed.). Scotts Valley, California: Create Space Independent Publishing Platform: ISBN-13: 978-1537473482.
2. Laane, J. (2017). *Frontiers and Advances in Molecular Spectroscopy* (1st ed.). Texas A&M University, USA: Elsevier Science, **ISBN:** 9780128112205.
3. Mohan, J. (2022). *Organic Spectroscopy: Principle and Applications* (4th ed). Kolkata: Narosa Publishing House Pvt. Ltd., ISBN-10: 8173195668.
4. Pavia, D.L., & Lapman, G.M. (2009). *Introduction to Spectroscopy* (4th ed.). Stamford, CT 06902 USA: Brooks/Cole Cengage Learning, ISBN-13: 9780495114789.
5. Silverstein, R.M., Webster, F.X. (2015). *Spectrometric Identification of Organic Compounds* (8th ed.). 111 River Street, Hoboken NJ 07300 US: John Wiley & Sons, ISBN 9780849390685.

Advanced Atomic Spectroscopy

Course Code: CHM-780

Credit Hours: 03

Pre-requisite: Nil

Objectives

- Present the comparison between the different atomic Spectroscopic techniques to find the best solution for analytical problem along with their use in numerous fields of application.
- Describe the latest developments in the field of flow injection and the Computer Management for laboratory automation.

Learning Outcomes

Students will have deep understanding of different types of atomic spectroscopy. Fundamental principles, instrumentation, and applications. Current challenges in atomic spectroscopy. Recent advancements and emerging technologies.

Course Outline

Unit 1. Overview of Analytical Techniques

Introduction to different analytical techniques. Importance of atomic spectroscopy in analytical chemistry. Review of atomic structure. Key concepts about atom and its nucleus. Fundamental concepts and importance of AAS in elemental analysis. Principles of absorption spectroscopy. BeerLambert Law and its application in AAS. Components of an AAS instrument.

Types of atomizers i.e., flame, graphite furnace.

Unit 2. Flame Atomic Absorption Spectrometry (FAAS)

Basic principle of flame atomization. Characteristics of different flames. FAAS Instrumentation, flame AAS setup and components. Light source, monochromator, and detector. Optimizing FAAS Conditions: Factors affecting sensitivity and precision. Flame temperature, burner height, and fuel/oxidant ratio.

Unit 3. Graphite Furnace Atomic Absorption Spectrometry (GFAAS)

Graphite Furnace Atomization: Principles of graphite furnace atomization. Advantages and limitations compared to flame atomization. GFAAS Instrumentation: Components of a GFAAS system. Heating cycle and temperature control. Optimizing GFAAS Conditions:

Temperature program optimization. Sample introduction techniques.

Unit 4. Sample Preparation Techniques

Sample Introduction: Techniques for introducing samples into the AAS instrument. Nebulization, sample injection, and hydride generation. Matrix Effects and Interferences:

Understanding matrix effects in AAS. Strategies for minimizing interferences.

Unit 5. Flame Atomic Emission Spectrometry (FAES)

Flame Atomization and Excitation: Principles of flame atomization and excitation. Flame characteristics and temperature control. FAES Instrumentation: FAES setup and components. Light source, monochromator, and detector. Optimizing FAES Conditions: Factors affecting sensitivity and precision. Flame temperature, burner height, and fuel/oxidant ratio.

Unit 6. Inductively Coupled Plasma-Atomic Emission Spectroscopy (ICP-AES)

Introduction to ICP: Principles of ICP and its advantages. Plasma generation and stability. ICP-AES Instrumentation: ICP-AES setup and components. Optical and detection Systems. Optimizing ICP-AES Conditions: Factors influencing analytical performance. Plasma power, nebulizer flow rate, and viewing height.

Unit 7. Inductively Coupled Plasma-Mass Spectrometry (ICP-MS)

Introduction to ICP-MS. Importance of ICP-MS in elemental analysis. Basic Principles of ICP-MS: Principles of inductively coupled plasma and mass spectrometry. Ionization processes and mass separation. Instrumentation Overview: Components of an ICP-MS instrument. ICP generation, mass analyzers, and detectors. ICP Source and Plasma Characteristics: Generation and optimization of the ICP. Plasma stability and tuning. Mass Analyzers in ICP-MS.

Recommended books/reference material

1. Bernhard W., Michael S. (1999). Atomic Absorption Spectrometry, 3rd Edition, Completely Revised Edition. ISBN: 978-3-527-28571-6.
2. Douglas A. Skoog, F. James Holler, Stanley R. Crouch. (2017). Principles of Instrumental Analysis. Published by Cengage Learning.
3. Robert T. (2024). Practical Guide to ICP-MS and Other Atomic Spectroscopy Techniques (4th ed.). Published by CRC Press.
4. Sune S. (2022). Atomic and Molecular Spectroscopy. Published by Springer.
5. Evans, E.H. (1998). Analytical Atomic Spectrometry. John Wiley & Sons Ltd. Baffins Lane, Chichester West Sussex PO19 1UD, England. ISBN: 0-471974188
6. Fifield, F. W., & Kealey, D. (2000). Principles and Practice of Analytical Chemistry. Blackwell Science Ltd. ISBN: 0-632-05384-4
7. Rita K. (2015). Atomic and Molecular Spectroscopy: Basic Concepts and Applications Cambridge University Press. ISBN: 9781107479999.

Sustainable Environmental Chemistry

Course Code: CHM-781

Credit Hours: 03

Pre-requisite: Nil

Objectives

The students will be able to develop/understand the

- Study the environmental pollution and interaction of pollutants with materials □
Dispose the nuclear waste and its proper management
- Experimental techniques for environmental monitoring.

Learning Outcomes

- Students will have deep understanding of sustainable chemistry.
- They will have command to understand Different Management Tools to Maintain/Sustain healthy environment.

Course Outline

Unit 1. Introduction to Sustainable Environmental Chemistry

Definition and fundamental concepts of Sustainable and Environmental Chemistry. Natural/Renewable Resources Depletion and Challenges Faced.

Introduction to Environmental Pollution including water and Soil Pollution.

Unit 2. Greenhouse Effect

Fundamental Concepts of Greenhouse Effect. Greenhouse gases and their effect on environment and habitats. Classification of Atmosphere and Ozone Layer Depletion Caused by Greenhouse Effect. Particulate Matter and their ultimate effect on the

Environment

Unit 3. Mechanism of Pollutants Reactions

Fundamental Principals about the Reactions Caused by the Pollutants. Various types of Pollutants interaction with materials both at Molecular level and Atomic Level and the Chemistry lying behind these interactions.

Unit 4. Gaseous/Nuclear/Particulate Matter Emissions and Their Management

Nox emission from industrial processes. Sources and Process Involving Aerosol production, Type and Classifications of Industrial Waste. Recyclable Industrial Waste including Chemical Waste. Nuclear waste and its management.

Unit 5. Kinetics and Thermodynamic Aspects

Chemical Kinetics Involved in the Environmental Chemistry and its role in the Sustainability. Thermodynamic aspects of atmospheric phenomena Atmospheric Chemistry, Importance of Clean energy Resources for future Challenges.

Experimental techniques for environmental monitoring.

Unit 6. Nuclear Waste and Hazard Management

Introduction to Nuclear Waste Management. Overview of nuclear waste types and sources Classification of nuclear waste: low-level, intermediate-level, and high-level waste environmental and health impacts of nuclear waste. Regulatory Framework for Nuclear Waste Management International and national regulations and standards licensing and permitting processes for nuclear waste facilities. Role of regulatory agencies and oversight bodies. Storage and Transportation of Nuclear Waste. Disposal of Nuclear Waste. Radiation Protection and Safety Measures. Stakeholder Engagement and Public Awareness.

Recommended Books/reference material

1. Artiola, J. Pepper, I. L. & Brusseau, M. L. (2004). *Environmental monitoring and characterization*. (1st ed.). Academic Press. ISBN: 978-0120644773
2. Baylisis, C. & Langlev, K. (2003). *Nuclear decommissioning, waste management, and environmental site remediation*. (1st ed.). ButterworthHeinemann. ISBN: 9780750677448.
3. Eckenfelder, W. W. & Englande, A. Jr. (2008). *Industrial water quality*. (4th ed.). McGraw-Hill Education. ISBN: 978-0824799489
4. Hites, R. A. (2012). *Elements of environmental chemistry*. (2nd ed.). Wiley. ISBN: 9781118041550
5. Overway, K. S. (2017). *Environmental chemistry: an analytical approach*. (1st ed.). Wiley. ISBN: 978-1118756973
6. Ramasami, Ponnadurai. (2023). *Sustainable Chemistry Research: Chemical and Biochemical Aspects*, Berlin, Boston. Published by De Gruyter.
7. Sankar P. D, Nayim S. (2021). *A text book of green chemistry*. Published by Techno World.

Solar Cell Chemistry

Course Code: CHM-782

Credit Hours: 03

Pre-requisite: Nil

Objectives

Understanding the principles of photovoltaic conversion:

- Students should grasp the fundamental concepts behind the conversion of sunlight into electricity, including the underlying chemical processes involved in solar cell operation.
- Knowledge of semiconductor materials: Gain an understanding of the properties of semiconductor materials commonly used in solar cells, including their electronic structure, bandgap, and optical properties. **Learning Outcomes**

The students will be able to

- Study and apply the Photovoltaic cell to generate the power
- Fabrication and characterization of different types of solar cells

Course Outline

Unit 1. Photovoltaics

Photovoltaic effect, Principle and working of solar cell, Photovoltaic cell and the power generation, efficiency of solar cell, Donors/acceptor materials and charge transport.

Unit 2. Polymer-Based, Inorganic, Organic and Hybrid Materials

Polymer-based, inorganic, organic and hybrid materials, New low band conducting materials, Donor/acceptor Interface, Transport layers, PEDOT-type material and its application in solar cells, Current equations in terms of drift and diffusion, Validity of the Drift-Diffusion equations, current equations for non-crystalline solids. Work function and the origin of Photovoltaic action.

Unit 3. Metal-Semiconductor Junction

Metal-semiconductor junction, semiconductor-semiconductor junction, electrochemical junctions and junctions in organic materials, Silicon-based solar cells.

Unit 4. Thin Film Solar Devices

Thin film solar devices, methodologies and development, (CuInSe₂ and CdTe etc), Organic and Hybrid solar cells, Photo-electrochemical devices and the concept of dye sensitization, Bulk heterojunction solar cells.

Unit 5. Devices Characterization

Performance and morphology of the device, Electrodes and Substrates requirements for organic photovoltaics, Barrier films, current approaches and recent trends.

Unit 6. Industrial and Research Application

Advanced research in the field of Photovoltaics. Research of photovoltaics Emerging trends and advanced applications.

Recommended books/reference material

1. Arkhipov, V. and Poortmans, J., (2006). *Thin film solar cells: fabrication, characterization and applications*. (1st ed.). Wiley.
2. Balzani, V., Credi, A., and Turro, N. J. (2021). *Solar Energy Conversion: Chemical Aspects*. Wiley Publisher.
3. Brabec, C., Dyakonov, V and Scherf, U. (2014). *Organic photovoltaics: materials, device physics, and manufacturing technologies*. (2nd ed.). WileyVCH.
4. Centi, G., Lemonidou, A. and Maji, T. K., (2022). *Solar Chemical Reactors: Materials, Design, and Applications*. Wiley Publisher.
5. Chiras, D. (2016). *Power from the sun: a practical guide to solar electricity*. (2nd ed.). New Society Publishers.
6. Corkish, R., Green, M. A., Sproul, A. Wenham, S. R., and Watt, M. E., (2013). *Applied photovoltaics*. (3rd ed.). Routledge. ISBN: 978-1849711425.
7. Fraas, L. M., & Partain, L. D. (2010). *Solar cells and their applications*. (2nd ed.)Wiley.
8. Jeyraj, A., Pandey, A. K., Rahim, N. A., & Selvaraj, L., Tyagi, S. K., Tyagi, V. V., (2016). *Recent advances in solar photovoltaic systems for emerging trends and advanced applications*. Renewable and Sustainable Energy Reviews, 53.

Advanced Solution and Colloidal Chemistry Course

Code: CHM-783

Credit Hours: 03

Pre-requisite: Nil

Objectives

Understanding the principles and applications of solution and colloidal systems: Students will gain an in-depth understanding of the behavior of colloidal systems, including the stability, aggregation, and phase behavior of colloidal particles in various solvent environments. They will also explore the practical applications of colloids in fields such as pharmaceuticals, cosmetics, materials science, and environmental remediation. Mastery of advanced experimental techniques for colloidal and solution characterization.

Learning Outcomes

The students will be able to

- Study the structure and characterization of different solvent and solvates
- Equilibrium in solutions and Deep Eutectic Solvents

Course Outline

Unit 1. An Overview of Solutions

Classification, importance and applications of different solutions in the chemistry, industry and life science, multicomponent systems; preferential solvation, Solvents characterization; microscopic structure of solvent and solvates; pair distribution function (PDF) and its determination using different techniques (spectroscopy and diffraction).

Unit 2. Molecular Dynamics and Microscopic Structure

Molecular dynamics and microscopic structure; different techniques of molecular dynamical calculations, Theories and laws related to solutions. Deep Eutectic Solvents, Transport properties; thermodynamics of solution; equilibria in solutions.

Unit 3.

Colloids and Surfactants

Spreading phenomenon; work of adhesion and cohesion; adsorption from solution; Gibbs adsorption equation, Surface tension and Young's and Kehrle equations, Molecular assemblies and insoluble surface mono layers, Langmuir Blodgett films, surface presence area diagrams.

Unit 4. Micellar Structures and Properties

Micellar structures and properties; micellar catalysis; bilayers and vesicles; membranes; micro- and macro emulsions; colloidal dispersions, Colloidal stability and DLVO theory.

Unit 5. Electro Kinetics

Electro kinetics-zeta potential and electrophoresis, Light scattering techniques; coagulation and flocculation.

Unit 6. Introduction of Ionic Liquids

Introduction, micellization behavior and application.

Recommended books/reference material

1. Adamson, A. W. & Gast, A. P. (2012). *Physical chemistry of surfaces*. (6th ed.). Wiley India.
2. Birdi, K. S. (2009). *Surface and colloid chemistry: principles and applications*. (1st ed.). CRC Press.
3. Butt, H. J. & Kappl, M. (2010). *Surface and interfacial forces*. (1st ed.). WileyVCH.
4. Butt, H. J., Graf, K., & Kappl, M. (2013). *Physics and chemistry of interface*. (3rd ed.). Wiley-VCH.
5. Koga, Y. (2017). *Solution thermodynamics and its application to aqueous solutions: a differential approach*. (2nd ed.). Elsevier Science.

6. Kontogeorgis, G. M. & Kiil, S. (2016). *Introduction to applied colloid and surface chemistry*. (1st ed.). Wiley.
7. Kumar, H. Sharma, P., & Sharma, S., (2023). *Introduction to ionic liquids, applications and micellization behaviour in presence of different additives*. Journal of Molecular Liquids, 123447.
8. Poling, B. E., Prausnitz, J. M., & O'Connell, J. P. (2001). *The properties of gases and liquids*. (5th ed.). McGraw-Hill Education.
9. Reichardt, C., & Welton, T. (2011). *Solvents and solvent effects in organic chemistry*. (4th ed.). Wiley-VCH.
10. Trémillon, B. (2012). *Chemistry in non-aqueous solvents*. Springer Science & Business Media.
11. Volkov, A. G. (2009). *Liquid interfaces in chemical, biological and pharmaceutical application*. (1st ed.). Dekker.

Thermodynamic Aspects of Catalysis

Course Code: CHM-784

Credit Hours: 03

Pre-requisite: Nil

Objectives

The students will be able to describe thermodynamic aspects of an interface. They will be capable to explain solid-liquid interface, catalyst preparation and their applications.

Learning Outcomes

The students will be able to

- Study thermodynamics of an interface
- Explain solid-liquid interfaces
- Apply catalytic preparation techniques and their applications in different synthetic processes.

Course Outline

Unit 1. Nature and Thermodynamics of Interfaces

Thermodynamic description of an interface; Gibbs-Duhem equation for an interphase, Gibbs adsorption isotherm, adsorption from solutions (dilute, liquid mixtures, nonelectrolytes, electrolytes, etc.) at solid-liquid interface.

Unit 2. Statistical Thermodynamics

Detergency and flotation, Kelvin's and Laplace equations, Partition distribution function, Maxwell-Boltzmann statistics.

Unit 3. Synthesis of Catalysts

Catalyst preparation techniques and their commercial utilization. Catalytic reactors.
Supported metal catalysts.

Unit 4. Catalytic Applications

Applications of heterogeneous catalysts, Catalysis for steam-reforming, CO- & CO₂methanation; water-gas shift; Fischer-Tropsch synthesis reactions.

Unit 5. Industrial Applications of Catalysis

Catalytic study for the syntheses of Ammonia, Nitric Acid, Sulfuric Acid, and chemical fertilizers etc, CO₂ capturing.

Recommended books/reference material

1. Adamson, A. W., & Gast, A. P. (2012). *Physical chemistry of surfaces*. (6th ed.). Wiley India.
2. C.K.F. Monguen, D Yu, OB Ayodele, S Daniel, ZY Tian. (2022). *Progress in catalysis for industrial applications*. Engineered Science, 20, 47-79.
3. Erbil, H. Y. (2006). *Surface chemistry of solid and liquid interfaces*. (1st ed.) WileyBlackwell.
4. Hanefeld, U., & Lefferts, L. (Eds.). (2018). *Catalysis: An Integrated Textbook for Students*. (1st ed.). Wiley-VCH.
5. Lowell, S (2011). *Powder surface area and porosity*. Springer.
6. Somorjai, G. A., & Li, Y. (2010). *Introduction to surface chemistry and catalysis*. (2nd ed.). Wiley.
7. Sun, S., Li, H., & Xu, Z. J. (2018). *Impact of surface area in evaluation of catalyst activity*. Joule, 2(6), 1024-1027.
8. Thomas, J. M., & Thomas, W. J. (2015). *Principles and practice of heterogeneous catalysis*. (2nd ed.). Wiley VCH.