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INTRODUCTION

The Department of Chemistry, Forman Christian College, A Chartered University (FCC), is committed to the goals and visions of the University in formation of a liberal arts curriculum, in pursuit of academic excellence and in development of strong moral values in its students to be of service to the peoples of Pakistan and the world community. Through its baccalaureate and M.Phil programs the Department provides an environment which nurtures and develops creative thought and critical understanding as students prepare to become scientists, teachers or innovative researchers.

Chemistry is a central science providing a foundation for students and researchers in essentially all areas throughout science and technology. It is thus essential for FCC to develop and maintain a sound and progressive Chemistry Department. The Department envisions a vital role in the economic and industrial developments in Pakistan. It plans to engage with local, national, and international chemistry communities through mutually beneficial scientific activities.

The Chemistry Department promotes the advancement of basic education in all major areas of chemistry including organic, inorganic, physical, analytical, and bio-related chemistries. Students are encouraged to apply their educational training and personal interests through innovative research projects. The Department engages in sound educational and research activities through development of up to date programs which will meet the current and future needs of the chemistry industry in Pakistan.

The Department pledges to become one of the top Chemistry Departments in Pakistan. Through its sound and innovative educational curriculum and research programs students will become Pakistan’s leaders in directing changes in the chemistry profession necessary for economic growth in the rapidly changing world community.

Strength of academic departments begins with faculty. Energized, forward-thinking staff devoted to academic excellence and visionary approaches to education and research are the core and essential features of a sound and progressive department.

Recruitment and retention of quality faculty is essential to Department development. The Chemistry Department has recruited faculty members with expertise in the full range of Chemistry areas. The faculty is a mixture of seasoned, veteran educators as well as young, talented and enthusiastic members. This combination will provide both sound direction as well as visionary growth to the Department.

Located in the newly built Armacost science building, the department has four large teaching laboratories and six postgraduate laboratories for research. New instruments include: atomic absorption spectrophotometer, digital polarimeter, thermogravimetric analyzer, CHNS/O analyzer, GC, gas chromatography-mass spectrometer (GC-MS), high performance liquid chromatography (HPLC), FT-IR spectrophotometer, UV-VIS spectrophotometers and Gamray electrochemical equipment.

A strong education and research agenda must attract quality students in both the baccalaureate and graduate programs. The Chemistry Department is strongly focusing on:
- Development of a strong, innovative, disciplined and well-rounded basic curriculum in all major areas of Chemistry
- Design curriculum to meet future goals of students in employment as well as in advanced education
- Encourage baccalaureate students to continue advanced education in the Chemistry Department, FCC
- Train students to be leaders, not simply laborers, in their respective fields of endeavor
- Development of a strong research Department program for both baccalaureate and M.Phil students; acquisition of up to date research equipment and supplies; establish research collaborations with prominent scientists in Pakistan and throughout the world
- Availability of financial resources through research grants and philanthropy
- Promote interactive student research groups
- Establishment of an active seminar program with students, faculty, and importantly, with outside scientists

A progressing and viable Department must have sound curriculum for both baccalaureate and MPhil programs. At FCC, designing and updating of curriculum is an ongoing process, and the Department has organized its curriculum to meet the requirements of a basic Chemistry education and within the guidelines mandated by the Higher Education Commission, Pakistan, and trends followed by major universities of Pakistan. In addition, the Department of Chemistry is committed to acquire and maintain international standards in terms of content, pedagogy and practices. The Chemistry Department has organized an Advisory Board composed of experts in Chemistry education and research. Most are senior directors of companies from the Chemical industry in Lahore. They have been instrumental in providing advice in structuring our educational and research programs to meet the growing and changing needs for trained chemists.

The booklet in your hand presents a somewhat detailed description of the courses of BS (Hons.) chemistry. The courses have been designed in a manner that after graduating in chemistry from FCC, a student must have an adequate mastery on the major areas of the subject.
ACKNOWLEDGEMENT

The detailed description of the courses that Department of Chemistry offers is the outcome of a lot of effort and hard work by our faculty. The description not only explains the details of the topics covered in our theory classes but also the lab activities related to each course. It was not an easy task. All of our faculty members devoted much time and effort to accomplish it. While the curriculum recommended by HEC, Pakistan, served as a strong baseline for this course description, the syllabi of some of the reputed national and international universities were also kept in view.

I take this opportunity to express my deepest gratitude for all of my colleagues at the Department of Chemistry for their cooperation. Without the collaboration of each one of them, the preparation and “synthesis” of this booklet was not possible. I particularly commend the meticulous efforts of our students’ handbook committee headed by Dr. Seemal Jelani. Their continuous efforts to coordinate with the faculty members, collect, and organize the data deserve special appreciation. I also appreciate our TA Anum Hayat for all the hard work she put to compile and arrange this booklet in its present form.

It is hoped that this detailed course description will serve as a guideline for our students and will provide our faculty a foundation for their continuous efforts to redesign and update our syllabus fulfilling both the national and international requirements.

Dr Dildar Ahmed
Chairperson,
Department of Chemistry
STUDENT LEARNING OBJECTIVES (SLOS)

OF

CHEMISTRY DEPARTMENT

Students majoring in Chemistry are expected to have an adequate mastery on the subject, think critically, know how to use their knowledge to solve problems, and are lifelong learners. They are specifically expected to:

- Explain major Chemistry concepts, laws and theories with suitable examples.
- Think critically while using chemistry concepts.
- Describe the range of career possibilities with training in Chemistry.
- Efficiently use library resources and electronic technology to gather information and solve problems.
- Apply ethical principles in the domain of Chemistry.
# Roadmap for Students Majoring in Chemistry

## Freshman Year

<table>
<thead>
<tr>
<th>General Education</th>
<th>As given in University road map</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>It is recommended that the students take the following courses preferably in the freshman year or if fails to take any of these, complete it in the subsequent year. CHEM 150, CHEM 160, CHEM 170</td>
</tr>
</tbody>
</table>

## Sophomore Year

A student opting Chemistry Major is strongly advised to make his/her plan of studies in consultation with his/her major advisor / Head of the Department.

<table>
<thead>
<tr>
<th>General Education</th>
<th>As given in University road map</th>
</tr>
</thead>
<tbody>
<tr>
<td>Major</td>
<td>It is recommended that a student take at least three or preferably four courses out of the following course during the Sophomore Year. CHEM 260, CHEM 250, CHEM 270, CHEM 271, CHEM 261</td>
</tr>
</tbody>
</table>

## Junior Year

<table>
<thead>
<tr>
<th>General Education</th>
<th>As given in University road map</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>By the time a student completes his/her Junior Year, he/she is expected to have studied the following courses: CHEM 311, CHEM 320, CHEM 330, CHEM 350, CHEM 361, CHEM 370</td>
</tr>
</tbody>
</table>

## Senior Year

Students should study as many courses as he/she can from his/her area of specialization, and must select at least ONE course from each of the remaining fields. Student must not forget to take the core course that was yet to be studied.
<table>
<thead>
<tr>
<th>Inorganic/Analytical Chemistry</th>
<th>Organic Chemistry</th>
<th>*Physical Chemistry</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHEM 454: Inorganic Electronic Spectroscopy</td>
<td>CHEM 465: Natural Products and Medicinal Chemistry</td>
<td>CHEM 473: Surface and Solid State Chemistry</td>
</tr>
<tr>
<td>CHEM 455: Inorganic Reactions Mechanism</td>
<td>CHEM 430: Chemical Principles in Biology</td>
<td></td>
</tr>
</tbody>
</table>

* Note: Those who intend to pursue their specialization in Physical Chemistry are required to take MATH 102 or MATH 201.

**Requirements for Major:** A student majoring in Chemistry is required to complete at least 48 credit hours courses of Chemistry including the following core courses: CHEM 250, 261, 270, 311, 320, 330, 350, 361, 370.

**Supporting Courses for Chemistry Major:** Relevant courses of MATH, STAT, PHYS & BIOT are advised.
COURSE DESCRIPTION

CHEM 100: INTRODUCTION TO CHEMISTRY

1. INTRODUCTION TO CHEMISTRY
   • Matter and its types
   • Atoms, Ions, Molecules
   • Elements, symbols, atomic mass, atomic number
   • Molecular formula
   • Mixture and Compound
   • Mixture and its types
   • Physical and chemical changes

2. INTRODUCTION TO VARIOUS BRANCHES OF CHEMISTRY
   • Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Analytical Chemistry,
     Biochemistry, Environmental Chemistry, Applied Chemistry, Material Chemistry, Green
     Chemistry.

3. ATOMIC STRUCTURE
   • General concepts, Bohr’s atomic model, orbital concept and electronic configuration.

4. THE PERIODIC TABLE
   • Modern periodic table and its features

5. FUNDAMENTAL CONCEPTS AND THEIR APPLICATION IN DAILY LIFE
   • Facts, laws, theories, scientific method
   • Units of measurement; SI units
   • Density, Specific gravity
   • Avogadro’s number, concept of mole
   • Concentration and its units
   • Qualitative and quantitative analysis

6. LEWIS STRUCTURES
   • Structures of polyatomic ions and molecules, importance of Lewis formula.

7. CHEMICAL NOMENCLATURE
   • How to name different chemical compounds, organic, inorganic; different systems of
     nomenclature,
8. CHEMICAL REACTIONS
   - Chemical reactions and their types
   - Chemical equations

9. STOICHIOMETRY
   - Balancing chemical equations
   - Limiting reactants
   - Percent composition
   - Empirical and molecular formulas

10. ACID-BASE CHEMISTRY
   - Concepts of acids and bases
   - Degree of dissociation
   - Salts and acid-base reactions
   - Acid-base character
   - Acid-base titrations
   - pH and ionization of water

CHEM 100: LAB ACTIVITIES
   - Apparatus in chemistry laboratory
   - Precautionary measures for laboratory/safety rules
   - Separation of two solids by sublimation
   - Separation of two immiscible liquid
   - Purification of water by distillation
   - Determination of melting point
   - Determination of boiling point
   - Separation of a mixture of inks by chromatography
   - Determination of pH of given solutions
   - Determination of the percentage of CH$_3$COOH in vinegar
   - Determination of percentage purity as well as impurity of the washing soda sample by volumetric method
   - Determination of purity of FeSO$_4$.7H$_2$O in its samples by volumetric method
   - Determination of the percentage of each component in the mixture containing HCl and NaCl dissolved/dm$^3$

CHEM 150: INTRODUCTION TO INORGANIC CHEMISTRY

1. ELECTRONIC STRUCTURE OF ATOMS & MOLECULES
   - Pauli exclusion principle, Aufbau principle & Hund’s rule
   - Atomic subshell energies and electron assignments
   - Electron configuration of the main group elements
• Electron configuration of the transition metals
• Electron configuration of the lanthanides & actinides
• Electron configuration of ions
• Electronic structure of molecules
• Periodic law
• Periodic tables
• Quantum numbers

2. MODERN THEORIES OF BONDING
• Valence bond theory
• Hybridization of orbitals
• Molecular orbital theory (MOT)
• Comparison of valence bond and molecular orbital theories
• Werner’s theory
• Crystal field theory
• Three center bonds
• Bonding theory of metals and intermetallic compounds
• Bonding in electron deficient compounds
• Hydrogen bonding

3. SHAPES OF MOLECULES
• Valence shell electron pair repulsion concept
• Applications of VSEPR concept
• Dipole moment

CHEM 150: LAB ACTIVITIES

• Solution Making
  a. Making solutions of given solids and liquids
  b. Making solutions of various concentrations
  c. Making dilutions from stock solution

• Volumetric Analysis
  a. Standardization of different solutions
  b. Determination of percentage purity and impurity of given solutions
  c. Determination of percentage composition of a given mixture
  d. Acid base titrations
  e. Redox/KMnO₄ Titrations
  f. Iodine Titrations

• pH Meter
  a. Calibration of a pH meter
  b. Determination of pH of orange juice by use of a digital pH/ion meter
CHEM 160 INTRODUCTION TO ORGANIC AND BIOCHEMISTRY

1. NATURE OF COVALENT BOND
   - Chemical bonding in organic molecules
   - Naming compounds and writing structural formulas
   - Properties of covalent compounds
   - Properties based on electronic structure and molecular geometry
   - Drawing Lewis structures of molecules and polyatomic ions
   - Diversity of organic compounds

2. ALKANES
   - Structure and nomenclature
   - Physical properties
   - Conformation of alkanes and cycloalkanes
   - Reactions of alkanes and cycloalkanes
   - Bond energies and modes of bond breakage
   - Free Radicals and photochemical reactions
   - Petroleum products

3. ALKENES AND ALKYNES
   - Structure and nomenclature
   - Physical properties
   - Geometric isomerism
   - Preparations of alkenes and alkynes
   - Addition reactions, their mechanisms and synthetic applications

4. AROMATIC HYDROCARBONS
   - Structure of benzene and concept of delocalization of electrons
   - Electrophilic substitution reactions
   - Orientation in benzene reactions, activating and deactivating groups and ortho/para and meta directing effect
   - Introduction to heterocyclic aromatic compounds

5. INTRODUCTION TO BIOCHEMISTRY
   - Introduction to biomolecules and its importance
6. **NUCLEIC ACIDS**
   - Structure of nucleic acids
   - Nucleosides
   - Nucleotides, DNA and RNA

7. **PROTEINS CHEMISTRY**
   - Amino acids as building blocks of proteins
   - Protein structure levels, primary, secondary and tertiary level of proteins structure
   - Enzymes and biocatalysis

8. **CARBOHYDRATES CHEMISTRY**
   - Classification, structure and functions of carbohydrates
     - a. Monosaccharide
     - b. Oligosaccharides
     - c. Polysaccharides
   - Chemical properties of monosaccharide and oligosaccharides

9. **MINERALS AND VITAMINS**
   - Minerals of nutrient importance
   - Role in transport proteins and enzymes
   - Important vitamins and their classification
   - Role of vitamins in metabolism

**CHEM 160: LAB ACTIVITIES**

- Qualitative organic analysis
  - a. Element detection
  - b. Functional group identification
  - c. Melting points of organic substances
  - d. Filtration techniques
- Crystallization technique
- Sublimation technique for purification
- Bromination of alkenes
- Nitration of phenol
- Biochemical tests
  - a. Tests for carbohydrates
  - b. Tests for proteins
  - c. Tests for lipids
CHEM 170: INTRODUCTORY PHYSICAL CHEMISTRY

1. THERMODYNAMICS
   - Basic Concepts
   - First Law of Thermodynamics
   - Thermochemistry and Thermochemical Calculations

2. QUANTUM THEORY AND ATOMIC STRUCTURE
   - Development of Quantum Theory
   - Wave – Particle Dualism & de Broglie Hypothesis
   - Bohr's Theory of Hydrogen Atom
   - Quantum Mechanical Model of Atom

3. STRUCTURE & PROPERTIES OF GASES
   - Properties of Gases, Gas Laws, Ideal Gas Equation,
   - Deviation from Ideal Behaviour, van der Waals Equation of State, Critical Phenomenon,
   - Postulates of Kinetic Molecular Theory of Gases, Derivation of Gas Laws from Equation of State of Gases, Concept of Average Kinetic Energy,
   - Graham's Law of Diffusion, Calculation of Molecular Speeds
   - Distribution of Molecular Speeds

4. INTERMOLECULAR FORCES
   - Properties of Solids & Liquids
   - Dipole – Dipole, Dipole induced Dipole and London Dispersion Forces, Hydrogen Bonding
   - Structure of Solids & Their Types
   - Crystal Structure & Packing Efficiency
   - Bragg's Law

5. CHEMICAL KINETICS
   - Differential and Integrated Rate Laws
   - Order of Reactions & Molecularity
   - Arrhenius Equation
   - Experimental Determination of Order of Reactions and Rate Constants
   - Elementary Description of Collision Theory of Reaction Rates

6. EQUILIBRIUM
   Chemical Equilibrium and Equilibrium Constants

7. SURFACE PHENOMENA
   Surface Energy, Surface Tension and Its Measurement
CHEM 170: LAB ACTIVITIES

- Calibration of volumetric apparatus
- Determination of heat of neutralization of strong acid with strong base
- Measurement of viscosity
- Surface tension measurements and parachor value of CH$_2$ group
- Study of kinetics of hydrolysis of an ester
- Measurement of refractive index of liquids and calculation of molar refraction
- Measurement of heat of solution
- Distribution constant of I$_2$ between water and carbon tetrachloride

CHEM 250: CHEMISTRY OF MAIN GROUP ELEMENTS

1. THE ALKALI METALS

- General characteristics and occurrence
- Uses and application of group II elements and their compounds
- Study of important compounds (Preparation, properties and applications) including, Lithium Carbonate, Lithium Hydroxide, Sodium Peroxide, Sodium Chloride, Sodium Nitrite, Sodium Nitrate, Soda, Sodium Cyanide, Sodium Tetraborate, Potassium Superoxide, Potassium Nitrate, Potassium Bromide, Potassium Iodide, Potassium Cyanide, Chrome Alum, Potassium Dichromate, Potassium Permanganate, Rubidium and Cesium compounds
- Complex compounds
- Diagonal behavior of Lithium with Magnesium
- Uses and application of group 1 elements and their compounds

2. THE ALKALINE EARTH METALS

- General characteristics and its occurrence
- Compounds of Beryllium, Magnesium, Calcium, Strontium, Barium and Radium
- Chelates and non-chelate complexes
- Diagonal behavior of Beryllium with Aluminum
- Uses and application of group II elements and their compounds
- Beryllium and Magnesium differ from other group members
- Comparison between alkali and alkaline earth metals

3. p- BLOCK ELEMENTS

- Properties and trends
- Boron and its occurrence
- Structure of diborane, B$_2$H$_6$
- Aluminum production, properties, uses and its compounds
- Electrolysis cell for Aluminum production
• Bonding in Al₂Cl₆
• Aluminum gemstones
• Carbon and its Inorganic compounds
• Sources and uses of carbon oxides
• Silicon and its compounds
• Silicate minerals
• Organosilicon compounds
• Common compounds of Tin and Lead
• Nitrogen compounds and Fractional distillation of air
• Phosphorus and its compounds
• Arsenic, Antimony, and Bismuth
• Oxygen and its oxides
• Sulfur, its occurrence and properties
• Structures of the Sulfate and Thiosulfate ions
• Selenium, Tellurium, and Polonium
• Sources and uses of halogens
• Standard electrode potentials of the halogens
• Oxyacids of the halogens
• Occurrence of the noble gases
• Properties and uses of noble gases
• Summary of concepts

CHEM 250: LAB ACTIVITIES

• Preparation of Sodium thiosulphate
• Preparation of Potash Alum
• Preparation of CuSO₄ from Cu turning
• Estimation of Lead as Lead Chromate in the given sample solution gravimetrically
• Estimation of Calcium in the given sample of CaCO₃
• Determination of NaCl in solution containing soda ash using Mohr’s method
• Determination of the number of x in CuSO₄.xH₂O by Iodometric titration
• Determination of amount of calcium and magnesium in the given sample of hard water
• Calibration curve of Na solutions by using flame photometer
• Determination of the quantity of Na in ppm by using flame photometer

CHEM 260: PRINCIPLES OF ORGANIC CHEMISTRY

1. RECALL BASIC CONCEPTS OF ORGANIC CHEMISTRY

• Nomenclature
  a. Nomenclature of organic compounds
  b. Structures and nomenclature of alcohols, phenols, ethers, thiols

• Review of hybridization
  a. sp³, sp², sp hybridization and structure
b. Lewis formulas and formal charge

- Polar and non-polar bonds and molecules, chemical polarity (Polarity of molecules, Polar molecules, non-polar molecules, bond dipole moments, covalent bond)

- Conjugated system
  a. Conjugated cyclic compounds (aromatic and non-aromatic compounds), common examples

- Resonance
  a. General characteristics of resonance
  b. Use of contributing structures
  c. Resonance hybrids
  d. Major and minor contributors (Rules)
  e. Resonance energy
  f. Resonance effect
  g. Examples

- Aromaticity, delocalization
- Inductive effect and examples
- Hyperconjugation

2. INTRODUCTION TO ISOMERISM AND ITS APPLICATION
- Structural isomerism (chain isomerism, positional isomerism, functional group isomerism, Tautomerism, metamerism)

3. STEREOCHEMISTRY
- Conformational analysis
- Geometric isomerism
- Optical isomerism, chirality, enantiomers, diasteriomers, racemic mixture, meso compounds, specific rotation, resolution of enantiomers

4. CHEMISTRY OF HYDROXYL CONTAINING COMPOUNDS
- Alcohols: Structure and Nomenclature
  a. Physical Properties of alcohols
  b. Preparation of monohydric alcohols
  c. Reactions of alcohol with metals and organic acids
  d. Oxidation of alcohols
  e. Polyhydric alcohols (Glycol, glycerol)
  f. Thiols
  g. Differences between primary, secondary and tertiary alcohols

- Phenols
  a. Structure and nomenclature
b. Physical properties and Preparation
c. Acidity of phenols

- Reactions of phenols
  a. Salt formation
  b. Ether formation
  c. Ester formation
d. Nitration
e. Halogenation
f. Friedel crafts reactions
g. Sulfonation
h. Carbonation
i. Formylation (Reimer Tiemann reaction)
j. Oxidation

- Ethers
  a. Nomenclature and preparation
  b. Physical properties
c. Cleavage of ether linkage
d. Autoxidation

CHEM 260: LAB ACTIVITIES

Experiments aimed at different laboratory techniques are arranged, such as recrystallization and melting points, boiling points, cooling, stirring, distillation, fractional distillation, vacuum distillation, steam distillation, filtration distillation, heating under reflux, drying, etc.

- Solvent Extraction technique
  a. Extractions using Separatory funnel

- Chromatographic techniques
  a. Paper chromatography (using dyes)
  b. Thin layer chromatography (Separation of spinach pigments by TLC)

- Preparation of ethyl benzoate and its IR analysis
- Functional group detection of alcohols and phenols
- Determination of optical activity on polarimeter
- Bromination of phenol

CHEM 261: ORGANIC CHEMISTRY I

1. INTRODUCTION TO ORGANOMETALLIC COMPOUNDS

- Organomagnesium and organolithium compounds
- Lithium di-organo-copper (Gilman) reagents
• Coupling reactions using transition metals catalyst, Heck, Stille and Suzuki reactions

2. HALOALKANES (ALKYL HALIDES)
   • Structure and nomenclature
   • Physical properties of haloalkanes
   • Preparation of haloalkanes by halogenation of alkanes
   • Mechanism of halogenation of alkanes, energy profiles
   • Regioselectivity of chlorination and bromination
   • Hammond postulate
   • Allylic halogenation, NBS bromination
   • Radical autoxidation and Radical addition of HBr to alkenes

3. NUCLEOPHILIC SUBSTITUTION AT SATURATED CARBON
   • Nucleophilic substitution in haloalkanes
   • Mechanisms of nucleophilic aliphatic substitution
   • Experimental evidence for SN1 and SN2 mechanisms
   • Analysis of several nucleophilic substitution reactions
   • 2-Elimination and mechanisms of 2-Elimination
   • Experimental evidence for E1 and E2 mechanisms
   • Substitution versus elimination
   • Analysis of several competitions between substitutions and eliminations
   • Neighboring group participation

• AMINES
   • Structure, nomenclature, classification, physical properties and preparation of amines
   • Chirality of amines and quaternary ammonium ions
   • Basicity and reactions with acids
   • Reaction with nitrous acid
   • Hofmann elimination
   • Cope elimination

CHEM 261 LAB ACTIVITIES

• Emphasis on lab safety precautions
• Preparation of lab report
• Expectations, and evaluation scheme
• Identification of the given organic compound: benzoic acid
• Preparation of a derivative of benzoic acid
• Identification of an aldehyde and preparation of its derivative when provided by glucose or benzaldehyde
• Identification of ketone and preparation of its derivatives (oxime or hydrazone) when provided by Acetone or acetophenone or benzophenone
• Identification of an ester hydrolysis or saponification reaction
• Qualitative analysis / identification of aldehyde and ketone by using Paper/TLC chromatography
• Separation of a mixture of volatile substances by GC-MS and its interpretation
• Identification and interpretation of functional groups by IR spectroscopy

CHEM 270: THERMODYNAMICS AND EQUILIBRIUM

1. BASIC DEFINITIONS
• Heat, Work, Energy, System, Surroundings, Transformation state, Thermodynamic function

2. FIRST LAW OF THERMODYNAMICS
• Reversible and irreversible processes
• Energy and the first law of thermodynamics
• Changes in state at constant pressure and the concept of enthalpy
• Constant volume processes
• Relation between \( C_p \) and \( C_v \)
• Adiabatic changes in state
• Dependence of enthalpy of a reaction on temperature
• Bond energies and bond enthalpies

3. SECOND LAW OF THERMODYNAMICS
• Concept of entropy
• Clausius inequality relation
• Entropy changes in isothermal processes
• Entropy as a function of temperature and volume, temperature and pressure
• Entropy changes in an ideal gas
• Third law of thermodynamics
• Entropy and probability

4. SPONTANEITY AND EQUILIBRIUM
• Gibbs Energy function and its properties
• Gibbs energy of real gases
• Temperature dependence of Gibbs energy
• Standard Gibbs energy of formation
• Helmholtz energy function
• Chemical potential
• Chemical equilibrium in a mixture of ideal gases and real gases
• Equilibrium constant and temperature dependence

5. PHASE EQUILIBRIUM
• Phase rule
• Clapeyron equation
• Solid-liquid, liquid-gas, solid-gas equilibria
• Integration of Clapeyron equation
• Solutions
  a. Ideal and non-ideal solutions
• Colligative properties
• Raoult's law
• Vapour pressure of solutions
• Osmotic pressure
• Depression of freezing point

CHEM 270: LAB ACTIVITIES
• Measurement of molecular weight of a compound by depression of freezing point
• Equilibrium constant of the reaction $\text{KI} + \text{I}_2 \leftrightarrow \text{KI}_3$
• Water – phenol phase diagram
• Determination of the molecular weight of a polymer by viscosity method
• Investigation of the Bronsted primary salt effect
• Specific rotation of sucrose and kinetics of hydrolysis of sucrose
• Association constant of benzoic acid in benzene
• Measurement of degree of dissociation of a weak acid
• Stoichiometry of a complex in solution by Job's method
• $pK_a$ value of an indicator by spectrophotometry method

CHEM 271: QUANTUM CHEMISTRY

1. BASIC MATHEMATICS
• Coordinate system
• Determinants and Vectors
• Complex numbers and operators
• Eigen value equation

2. DEVELOPMENT OF QUANTUM MECHANICS
• Atomic spectra and black body radiation
• Photoelectric effect
• Wave particle dualism
• Postulates of quantum mechanics
• Schrodinger equation
• Significance of wave function
• Application of postulates to simple systems
• Particle in a 1 – D box and a 3 – D box
• Energies and wave function
• Simple problems

3. HARMONIC OSCILLATOR
• Schrodinger equation and its asymptotic solution
• Vibrational energies and wave function
• Hermite polynomials
• Vibrational spectroscopy

4. RIGID ROTATOR
• Separation of variables
• Eigen values and eigen functions of rigid rotator
• Associated Legendre polynomials
• Rotational spectroscopy

5. HYDROGEN ATOM
• Schrodinger equation, Phi, R, and theta dependent equations and their solutions
• Radial wave function
• Lagurre polynomials
• Physical significance of hydrogen – like, wave functions

6. SOME FUNDAMENTAL THEOREMS OF QUANTUM MECHANICS

7. LADDER OPERATORS AND ELECTRON SPIN

CHEM 311: FUNDAMENTAL ANALYTICAL CHEMISTRY

1. BASIC PRINCIPLES OF SPECTROSCOPY

2. ULTRAVIOLET AND VISIBLE SPECTROSCOPY
• Electronic transitions and Beer’s law
• Quantitative calculations
• Organic molecules and Chromophores
• Transitions (n → σ *, n → π *, π → π *, σ → σ*)
• Use of ultraviolet spectra in structural determination
• Applications of UV/Visible spectroscopy
3. INFRA-RED SPECTROSCOPY
- Mechanics of measurement
- Vibrational energy levels
  a. Determine the kinetic and potential energy and the vibrational frequency of a harmonic oscillator
  b. Determine the force constants, vibrational frequencies and spacing between vibrational energy levels for various chemical bonds
  c. Determine the number of rotational, vibrational and translational degree of freedom for molecules
  d. Determination of infrared inactive vibrational modes
- Characteristic group absorptions of organic molecules
- Interpretation of infrared spectra

4. INTRODUCTION TO MS AND NMR SPECTROSCOPY
- MS instrumentation, ionization and detection techniques, proton NMR chemical shift and spin-spin coupling

5. ANALYTICAL OBJECTIVES
- Analytical Science
- Qualitative and Quantitative Analysis
- The analytical process
- Validation of a method
- Range – size of sample

6. GRAVIMETRIC AND VOLUMETRIC METHODS
- Preparation of standard base solution
- Preparation of standard acid solution
- Buffer
- Handling and treating samples
- Gravimetric analysis
- Obtaining the sample
- Operations of drying and preparing a solution of analyte

7. DATA HANDLING
- Accuracy and precision
- Determinate and Indeterminate errors
- Significant figures and rounding off data
- Statistical evaluation of data
- T-test and Q-test
- Correlation Coefficient

8. QUALITY ASSURANCE AND QUALITY CONTROL
- Quality Control
- Quality Assurance
- Laboratory Accreditation
9. COMPLEXOMETRIC TITRATION
10. REDOX TITRATION
11. NON-AQUEOUS TITRATION
12. KARL FISCHER TITRATION

CHEM 311: LAB ACTIVITIES

- Preparation of solutions in molarity, percentage composition (w/w and w/v) and ppm/ppb concentration terms
- Preparation of an acidic and a basic buffer solution
- Estimation of Lead as Lead Chromate in the given sample solution gravimetrically
- Estimation of Calcium in the given sample of CaCO₃
- Estimation of Manganese using EDTA
- Determination of the concentration of FeSO₄ solution by titrating against molar solution of KMnO₄
- Determination of the amount of NaCl in solution of commercial soda ash dissolved per litre using Mohr’s method when provided with molar solution of AgNO₃
- Determination of the number of x in CuSO₄ₓH₂O when provided with molar solution of Na₂S₂O₃ by Iodometric titration
- Determination of the concentration of given solution of KMnO₄ by using a UV-VIS spectrophotometer
- Determination of λ_max of a substance by colorimetric analysis
- Spectrophotometric determination of iron in given sample of drinking water
- Study of IR spectra of given compound and identification of major functional groups

CHEM 320: INDUSTRIAL CHEMISTRY

1. INTRODUCTION

- Basic concepts of industry, industrial production and quality issues
- Viable industrial methods

2. ORGANIC INDUSTRIES

- Production of methanol, formaldehyde, methyl amines and halogenated organic compounds, olefins and polymer industry associated with olefins
- Poly condensation polymers like polyester and polyamide (nylon) industry
- Pharmaceutical industry, scope, formulations and production
- Soap and detergents
- Paints and dyes
3. COMMON INDUSTRIES IN PAKISTAN

- Paper and pulp industry
- Glass industry
- Sugar and molasses industry
- Cement and ceramics industry
- Manufacturing of steel
- Refining of metals by extraction from respective ores
- Introduction to textile and leather industry and processes carried in them

CHEM 320: LAB ACTIVITIES

- Laboratory scale synthesis of common drugs like aspirin
- Simple radical and condensation polymers
- Synthesis and application of dyes and textile chemical
- Analysis of free base in soaps
- Acid and iodine values of fats/oils
- Determination of the components of cements

Besides, an educational trip to industry to get the know-how of the systems in industry is also arranged for the students of this course.

CHEM 330: BIOCHEMISTRY

1. CARBOHYDRATES

- Classification, Chemical properties and working with carbohydrates
- Monosaccharides, disaccharides and polysaccharides
- Glycoconjugates (proteoglycans, glycoprotein’s, and glycolipids)
- Carbohydrates as informational molecules (the sugar code)

2. PROTEINS

- Amino Acids as building blocks of proteins, their structures
- Synthesis of proteins
- Acid base properties
- Proteins, primary secondary and tertiary structure of proteins
- Structural aspects of important proteins like keratins
- Silk fibers
- Hemoglobin and myoglobin

3. LIPIDS

- Storage Lipids
- Structural lipids in membranes
- Lipids as signals, cofactors, pigments and working with lipids
• Fatty Acids, Triacylglycerols, Glycerophospholipids and Sphingolipidis
• Steroids, lipids bilayers and lipids mobility

4. NUCLEIC ACIDS
• Basic Nucleic Acid Structure
• Nucleic Acid Chemistry
• Other Functions of Nucleotides

5. ENZYMES NOMENCLATURE
• An introduction to enzymes
• Classification and naming enzymes
• Enzyme kinetics as an approach to understanding mechanism
• Examples of enzymatic reactions, regulatory enzymes

6. MECHANISM OF ENZYME ACTION
• Enzyme nomenclature
• Substrate specificity
• Cofactors and coenzymes
• Acid-base catalysis
• Covalent catalysis
• Metal ion catalysis
• Electrostatic catalysis
• Catalysis through proximity and orientation effects
• Catalysis by preferential transition state binding
• Enzymes structure and catalytic mechanism

7. ENZYME KINETICS
• Chemical Kinetics
• Enzyme Kinetics
• Analysis of Kinetic data
• Bisubstrate Reactions
• Competitive Inhibition, Uncompetitive Inhibition, Mixed Inhibition

CHEM 330: LAB ACTIVITIES
• Qualitative analysis of carbohydrates, proteins, and lipids
• Isolation of DNA from onion and its analysis
• Preparation of different buffers
• Titrations using amino acids
• Determination of isoelectric point
• Isolation of casein from milk
• Analysis of egg protein
• Determination of enzyme activity
• Study of enzymes kinetics

CHEM 350: COORDINATION CHEMISTRY

i. INTRODUCTION AND HISTORICAL DEVELOPMENT

• Introduction, nomenclature and historical development
• Werner and Jorgenson controversy

2. THE COORDINATE BOND

• The Electron – pair bond
• The Concept of Effective Atomic Numbers
• Lewis Acid-Base concept
• Electronic structure of the atom
• Valence Bond Theory
• Valence Bond diagrams of various metal complexes
• Magnetic properties of complexes
• Electrostatic Crystal Field Theory (CFT)
• High spin and low spin complexes
• CF diagram of octahedral
• Tetrahedral and square planar complexes
• Molecular Orbital Theory (MOT)
• Molecular Orbital diagrams of some diatomic molecules and some complexes

3. STEREOCHEMISTRY

• Geometry of coordination compounds, octahedral, tetrahedral, square planar, trigonal pyramid
• Valence shell electron pair repulsion theory
• Distortions in octahedral complexes due to presence of d-electrons
• Isomerism in metal complex
• Geometrical isomerism in octahedral and square planar complexes
• Isomerism with symmetrical bi-dentate and unsymmetrical bi-dentate ligands
• Optical isomerism in octahedral complexes
• Plane polarized light
• Levo and dextro isomers
• Trisbidentate and cis-bidentate optically active complexes complexes
• Dissymmetric complexes
• Optical Rotatory Dispersion(ORD)
• Circular Dichroism (CD)
• Other isomerisms like, coordination isomerism, ionisation isomerism, linkage isomerism

4. COMPLEX ION STABILITY
• Concept of stability and its importance
• Stability constants and its determination
• Factors that influence complex stability
• Stability constant of ML6 complexes Vs CFSE
• Size and charge effect
• Crystal field effects
• Chelate effect and Chelate ring size
• Hard and soft acids and bases

5. KINETICS AND MECHANISMS OF REACTIONS OF COORDINATION COMPOUNDS
• Importance of study of rate of reactions
• The rate law and rate of a reaction
• Effective collisions
• Inter and labile complexes
• Mechanisms of substitution reaction
• Octahedral and square planar substitution reaction
• Mechanism for redox reactions

CHEM 350: LAB ACTIVITIES
• Synthesis of copper ammine complex
• Gravimetric analysis of sulphate ion in the synthesized complex.
• Synthesis of trioxalato chromium(iii) complex.
• Synthesis of nickel dimethyl glyoxime complex
• Complexometric titration metal ions with EDTA
• Synthesis of [Co(en)₃]Cl₃
• Resolution of [Co(en)₃]Cl₃ into its isomers (cis, d, l)
• Stoichiometry (metal ligand ratio) of complexes Iron (ii) and 1-10 phenanthroline complex

CHEM 361: ORGANIC CHEMISTRY II

1. INTRODUCTION TO ORGANIC SYNTHESIS
• A review of various reactions in chemistry
• drug discovery, drug design and lead compounds
• Organic synthesis: basic concepts and scope; bond cleavage, nucleophiles, electrophiles and free radicals, lengthening and shortening of chain
• Functional groups inter conversions

ii. CHEMISTRY OF ALDEHYDES AND KETONES

• Detailed study of aldehydes and ketones
• Nucleophilic addition to carbonyl group
• Reactions of aldehydic and ketonic group
• Reduction and oxidation of carbonyl group
• Grignard reagents

iii. CHEMISTRY OF ENOLATES

• Enolates, reaction to carbon alpha to carbonyl group, Aldol condensation, Cannizaro reaction, Wittig reaction, Michael reaction
• Malonic ester synthesis, acetoacetic ester synthesis, Claisen condensation, Hell-Volhard-Zelinski reaction, Williamson ether synthesis, Baeyer-Villiger oxidation, imine formation

b. CHEMISTRY OF CARBOXYLIC ACIDS AND THEIR DERIVATIVES

• Study of carboxylic acids and their derivatives, preparations and reactions; synthetic applications
• Functional group protection, multifunctional compounds, functional-group compatibility, protection of aldehydes and ketones
• Real world examples of synthesis: synthesis of ibuprofen, ketoprofen, valium

CHEM 361: LAB ACTIVITIES

Experiments involving synthesis of different organic compounds, reflux, filtration and recrystallization techniques

• Preparation of acetonilide from aniline
• Preparation of phenyl-azo β-naphthol
• Preparation of azo dye of phenol and sulfanilic acid by diazotization
• Preparation of benzoyl glycine (synthesis of an amide)
• Preparation of cinnamic acid from benzaldehyde and malonic acid (knoevenagel reaction)
• Preparation of benzalnilide from benzoyl chloride using schotten –bauman reaction
• Preparation of benzanilide from benzoyl chloride using schotten –bauman reaction
• Preparation of benzophenone using zinc and acetic acid
• Preparation of dibenzalacetone from benzaldehyde and acetone

CHEM 370: KINETICS & MECHANISM
1. CHEMICAL KINETICS
   - First and second order reactions
   - Reaction mechanism
   - Unimolecular reactions
   - Complex and chain reactions
   - Theories of reaction rates
   - Fast reactions and reaction in solution

2. ELECTROCHEMISTRY
   - Electrode potential
   - Ion selective electrodes
   - Electrochemical cells
   - Measurement of electrode potential
   - Electrical work
   - Temperature dependence of cell potential
   - Electrolysis, polarography
   - Cyclic voltammetry
   - Impedance

CHEM 413: INSTRUMENTAL METHODS OF ANALYSIS

1. ATOMIC SPECTROSCOPY
   - Atomic Absorption Spectroscopy (AAS)
   - Theory and principle of atomic absorption
   - Atomic absorption spectrum of atoms
   - Difference of atomic and molecular spectrum
   - Instrumentation of Atomic Absorption Spectrophotometer
   - Advantages and applications

2. ATOMIC EMISSION SPECTROSCOPY
   - Theory and principle of atomic emission
   - Emission spectrum of atoms and flame emission spectroscopy
   - Instrumentation of flame emission spectrophotometer
   - Advantages and applications

3. THERMAL METHODS OF ANALYSIS
   - Theory, principle and working of Thermogravimetric Analysis (TGA), Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC)
   - Their Instrumentation And Applications
4. CHROMATOGRAPHIC SEPARATION TECHNIQUES
- Principle of chromatographic separation, concept of theoretical plates and height equivalent of theoretical plates (HETP)
- Different types of chromatography, paper chromatography, Thin Layer Chromatography (TLC), High Pressure Liquid Chromatography (HPLC), Gas Chromatography (GC), Gel Permeation Chromatography (GPC) or Size Exclusion Chromatography, electrophoresis
- Hyphenated techniques such as, LC-MS, LC-FTIR

5. MASS SPECTROMETRY
- Tandem MS, ion trap MS, Inductively Coupled Plasma MS (ICP-MS)
- Matrix Assisted Laser Desorption Ionization-Time Of Flight MS (MALDI-TOF MS)

6. INTRODUCTION TO NUCLEAR TECHNIQUES
- Neutron activation analysis
- Nuclear quadrupole resonance
- Isotope dilution method
- Isotope ratio MS
- Mossbauer spectroscopy
- Radio-immuno assay

7. X-RAY TECHNIQUES
- Production of X-rays
- Powder X-ray diffraction and single crystal XRD
- Advantages and applications

CHEM 413: LAB ACTIVITIES
- Determination of metals using AAS
- Determination of Ca in Milk by FES
- Determination if Na in drinking water
- TGA/DSC evaluation of Calcium carbonate
- Determination of purity of a compound using TGA/DSC
- Separation of a given mixture using TLC
- Separation and identification of different amino acids using paper chromatography
- Separation and analysis of a given mixture using HPLC
- Separation and analysis of a given mixture using GC/MS

CHEM 421: PHARMACEUTICAL CHEMISTRY
1. HISTORY OF PHARMACEUTICALS
   - Development of pharmacological principles of drugs
   - Classification of drugs on different bases
   - Paul Ehrlich’s importance
   - Early sulfa drugs

2. ANTI-BACTERIAL AND ANTI-VIRAL DRUGS
   - Mechanisms of action
   - Structures and selectivity

3. PHARMACODYNAMICS
   - Targets of human drugs
   - Transportation and Mechanisms of action

4. PHARMACOKINETICS
   - Absorption, distribution, metabolism, excretion; liver metabolism, pH, ionization; transport

5. SOURCES OF CHEMICALS FOR DRUG DISCOVERY
   - Natural products
   - Known chemicals
   - Individual synthesis
   - Combinatorial chemistry
   - Oligonucleotides
   - Peptidomimetics

6. DRUG/LEAD DISCOVERY
   - Target discovery in vitro and in vivo models
   - Assays and HTS

7. LEAD TO DRUG CHEMISTRY
   - Necessary chemical features of molecules for a drug
   - Functional groups prominent in known drugs
   - Lipinsky’s rules
   - Hammett equation
   - Lipophilicity
   - Partitioning
   - Isosteres and bioisosteres
8. SAR AND QSAR

- Computer based technology
- X-ray crystallography
- Chemical information on internet

9. FORMULATION

10. DELIVERY

11. REGULATORY APPROVAL AND CLINICAL TRIAL SUMMARY

CHEM 421: LAB ACTIVITIES

- Beer-Lambert law and spectrophotometric analysis of drugs
- FTIR and drug analysis
- Partition coefficient
- Polarimetry in drug quality control
- Pill structure and dissolution
- Chromatography – TLC and column for drugs
- Analysis of a drug by HPLC and GCMS
- Analysis of mineral elements in food/mineral supplements using Atomic Absorption spectrophotometer
- Determination of iron in iron pills
- Analysis of ascorbic acid in vitamin C tablets

Besides, a study trip of a pharmaceutical industry is arranged to familiarize students with different process and stages of drug manufacturing.

CHEM 430: CHEMICAL PRINCIPLES OF BIOLOGY

- Energetics and thermodynamics of cell functions
- Water chemistry in the living system
- Cell control mechanisms
- Cell signaling
- Hormones, their chemistry and roles
- Growth and metabolism
- Chemistry involved in different metabolic processes
- Structure and role of DNA, RNA
- Discussion on topics like
  a. GPCR; PKA and PKC
  b. Tyrosine kinase/phosphatase
  c. PI3 Kinase, PKB
  d. Apoptosis
  e. Cell division
CHEM 430: LAB ACTIVITIES

Experiments are arranged using chromatography and electrophoresis; isolation and analysis of proteins, and enzymatic action.

- Initial stages of protein purification
- Gel electrophoresis
- Column chromatography for protein analysis
- Enzymatic assays

CHEM 440 ENVIRONMENTAL CHEMISTRY

1. INTRODUCTION, SCOPE AND IMPORTANCE

- Concept of environment and its sustainability
- Generation and fate of common chemical pollutants
- Toxicity and issues related to industrial waste
- Fossil fuels and impacts on ecosystems
- Human activity and environment
- Role of chemistry

2. WATER POLLUTION AND NOISE POLLUTIONS

- Physical properties of water
- Contaminations in water particular emphasize on transition metal and volatile organic components
- BOD and COD tests for water
- Effect of pesticides, herbicides and surfactants on water
- Treatment of water for removal of above mentioned contaminations
- Sound and noise and factor maintained for reducing the noise pollutions (like public awareness etc.)

3. AIR AND LAND POLLUTION

- Atmosphere and its different regions
- Essential ratios of gasses required for each region in atmosphere
- Green house effect and Emission of green house gases
- Acid rain
- Nitrogen cycles
- In land pollution basic contamination of agricultural land
- Acidity and alkaniity
- Essential organic fertilizers required for agricultural land
- Hazardous solid waste, issues and their solutions
- Urban waste management
4. ENVIRONMENT PROTECTION, NATIONAL AND INTERNATIONAL EFFORTS

CHEM 440: LAB ACTIVITIES

Experiments are arranged to analyse water, air and soil samples using AAS, gravimetric analysis, CHNSO analyzer etc. For example,

- Estimation of different transition metal ions in tap water and canal water by gravimetric analysis and its measurement by Atomic Absorption Spectroscopic
- Calculation of different ratios of carbon, nitrogen and sulfur by means of CHNSO analyzer in agricultural land

CHEM 442: GREEN CHEMISTRY

1. INTRODUCTION AND PRINCIPLES OF SUSTAINABLE AND GREEN CHEMISTRY

- Green chemistry and industry
- Waste minimization and atom economy
- Reduction of materials use and non-renewable raw material use
- Reduction of energy requirement
- Inherently safe design
- Alternative solvents

2. GREEN CHEMISTRY AND SUSTAINABLE DEVELOPMENT

- The concept of sustainability
- Green chemistry and sustainability parameters
- Sustainable use of chemical feedstock, water and energy
- Environmental resilience
- Life-cycle assessment (as a tool for identification of more sustainable products and processes)

3. INDUSTRIAL PROCESSES USING CATALYSTS

- Zeolite-based solid acid catalysts
- Hetero poly acid-based solid acid catalysts
- Sulfated zirconia
- Ion-exchange resins
- Acidic and pillared clays
- Silica nano composite
- High-octane fuels
- Waste minimization in industry (by means of purification, choice of starting material, yields, number and order of steps, robustness, solvents, reagents, reaction temperature, heavy metals, endurance etc.)
4. POLYMER-SUPPORTED REAGENTS
   - Polymeric tools for organic synthesis
   - Co-polymerization with usual Monomers (Polystyrenes, Polyacrylates, PolyVinylPyridines, Poly benzimidazoles, Poly phosphazenes, Chlorofluoro polymers)

5. BIOCATALYSIS
   - Chemical production by biocatalysis, (Pharmaceuticals, flavours and fragrance compounds, carbohydrates)
   - Biodesulfurisation

6. RECENT ADVANCES IN PHASE-TRANSFER CATALYSIS
   - Progress in classical PTC reactions
   - Nucleophilic aliphatic and aromatic substitutions
   - Phase-transfer catalysis elimination and isomerisation reactions
   - Base-promoted C, N, O and S alkylation and arylation reactions
   - Inverse PTC
   - Three liquid phases and triphase catalysis
   - Asymmetric PTC
   - Phase-transfer catalysis in polymerization processes
   - Applications of PTC in analytical chemistry
   - Phase transfer combined with metal catalysis
   - Phase transfer in homogeneous transition metal catalysis
   - Hydrogen peroxide and other PTC oxidations and halogenations
   - Supercritical and ionic liquid PTC

7. POTENTIAL CONTRIBUTIONS OF HYDROGEN PEROXIDE
   - Manufacture of hydrogen peroxide and its uses
   - Peroxygen systems and their reactivity
   - Effect of acids and bases
   - Oxygen species
   - Per-acids and organic activation
   - Enzymes and catalytic activation
   - Peroxo–metal systems

8. APPLICATIONS OF MICROWAVES FOR ENVIRONMENTALLY BENIGN SYNTHESIS
   - Background and properties of microwaves
   - Influence of microwave heating on chemical reactions
   - Rate studies and investigations into ‘microwave effects’
   - Approaches to microwave assisted organic chemistry
   - Solvent-free methods
• Methods with solvents
• Advantages of the pressurized microwave systems
• Elevated temperature and rapid heating
• Cooling, ease of use for high-temperature reactions and control of heating
• Exothermic reactions
• Differential heating and viscous reaction mixtures
• Reaction vessels
• Reactions with a distillation step
• Flexible operation high-temperature water as a medium or solvent for microwave-assisted organic synthesis
• Photochemistry
• Electrochemistry
• Fuel cells for greener chemistry applications

CHEM 442: LAB ACTIVITIES

• Water based organic synthesis
• PTC based transformations
• Microwave radiated reactions
• Synthetic route for different polymers using green resources
• Reaction involving renewable resources

CHEM 450: ADVANCED INORGANIC CHEMISTRY

• Characteristics of transition metals
• General chemistry of 1st transition series
• Nomenclature of coordination compounds
• Werner’s theory
• Chelates
• Transition metal complexes
• Valence bond theory
• Crystal field theory
• Molecular orbital theory
• Discussion on each element of 3d, 4d, 5d and 6d series
• Discussion on each element of lanthanide and actinide series
• Chemistry of nitrosyl and carbonyl compounds

CHEM 450: LAB ACTIVITIES

• Standardization of HClO₄
• Titration of a water insoluble base by perchloric acid
• Assay of ephedrine hydrochloride in tablets
• Preparation of sodium methoxide solution
• Standardization sodium methoxide solution
• Assay of allopurinol in tablets
• Preparation of CO₂ critical fluid
• Extraction of fragrances from flowers by use of CO₂ critical fluid
• Preparation of Ni(CO)₄

More experiments cannot be performed because of non-availability of lanthanide and actinide salts.

CHEM 453: CHEMICAL APPLICATIONS OF GROUP THEORY

• Group theory and examples of groups such as, humans, animals, birds, flowers etc.
• Symmetry elements and operations
• Classification of molecules into point groups
• Group representations
• Numerical representation of symmetry groups
• Bethe and Mullican representation of groups (A, B, E, T)
• Properties and characters of representations
• Properties of representations of groups
• Matrices & transformation matrices
• Group representations and character tables
• Reducible and irreducible representations
• Applications of group theory to bonding theories (valence bond theory, molecular orbital theory and crystal field theory)
• Chirality, and infrared spectroscopy

CHEM 454: INORGANIC ELECTRONIC SPECTROSCOPY

1. BRIEF INTRODUCTION OF:
• Structure of atom
• Quantum numbers
• Orbital angular momentum quantum number (l) and Magnetic orbital angular Q. Number (m_l)
• Spin quantum no. (s) and Magnetic spin Q. Number (m_s)
• Shapes of s, p, and d orbital
• Russel- Saunders coupling scheme
• L, S, J quantum numbers
• Microstates

2. CONFIGURATION
• Terms and Term Symbols
• Term diagrams in various symmetries
• Weak and Strong Field approach
• Term diagrams in lower symmetries
• Basis of Crystal Field Theory
• Crystal Field diagrams
• Crystal field stabilization energy

3. A BRIEF INTRODUCTION OF GROUP THEORY
• Symmetry, its operations and elements
• Symmetry of Atomic orbitals
• Point Groups and Group representations
• Reducible and irreducible representations
• Direct products

4. BASIS OF CRYSTAL FIELD THEORY
• Crystal Field diagrams
• Crystal field stabilization energy
• Energy calculations
• Ligand field diagrams in regular and in distorted fields
• Crystal field spectra of various transition metal complexes
• Energy level calculations
• Variation of the Racah parameter B
• The spectrochemical series
• Nephelauxetic Series

5. CORRELATION DIAGRAMS
• Tanabe-Sugano diagrams
• Selection rules
• Band intensities and band assignments

6. INTERPRETATION OF CRYSTAL FIELD SPECTRA OF VARIOUS METAL COMPLEXES
• d^1 to d^{10} cases
• Charge transfer spectra of low symmetry complexes

CHEM 455: INORGANIC REACTION MECHANISMS
• Kinetics and rate laws
• Types of reactions of complexes
• Inert and labile complexes
• Substitution reactions
• Dissociative mechanism
• Displacement mechanism
• Substitution reactions of octahedral complexes
• Base hydrolysis
• Anation reactions
• Substitution reactions without cleavage of the metal ligand bond
• Substitution reactions of square planar complexes
• Substitution reactions of trigonal bipyramidal complexes
• Isomerization reaction
• Stereochemical changes occurring during substitution reactions
• Substitution reactions involving stereochemical changes
• Reactions involving only stereochemical changes
• Intermolecular path, intramolecular mechanism
• Cis-trans isomerization
• Electron transfer
• Outer sphere and inner sphere mechanism
• Two electron transfer

CHEM 462: SPECTROSCOPY OF ORGANIC COMPOUNDS

1. IR SPECTROSCOPY
• Basic concepts
• Nature of radiation/light, its properties and various parameters.
• Application of infrared spectrophotometry in structure determination.
• Problems of functional group determination.

2. $^1$H NMR SPECTROSCOPY
• Basic Concept, magnetically active nuclei
• Discussion of proton NMR, a review of concepts and terminologies, Chemical Shift, Coupling constants, spin-spin splitting,
• Structure elucidation, structural Problems and how to solve them

3. $^{13}$C NMR
• Chemical Shift assignments, heteronuclear H-C systems,
• DEPT
• NOE and its significance
• Problems of structure elucidation using proton and C-13 NMR

4. TWO-DIMENSIONAL NMR, STATIONARY AND ROTATING FRAME OF REFERENCE, BEHAVIOUR OF MAGNETIZATION
• Correlation spectroscopy, COSY
• HETCOR, Use of spectra in structure elucidation
• Application of 2D NMR spectroscopy
• Recent advances in 2D NMR, problem solving

5. MASS SPECTROMETRY
• Ionization techniques, detection techniques, electron impact, chemical ionization
• MALDI
• Fragmentation patterns of different classes of organic compounds, McLafferty rearrangement
• Applications of mass spectrometry in structure elucidation

CHEM 462: LAB ACTIVITIES
Experiments are arranged to use UV-Vis spectrophotometer, IR spectrometer, and GC-MS. Examples:
• Determination of IR spectrum of an aldehyde, its derivatization and the IR spectrum of the product, and to compare the two
• Determination of IR spectra of a ketone and its derivative, of a carboxylic acid and its derivative, etc.
• Isolation of essential oils from a plant sample and their GC-MS analysis
• Experiments based on other available instruments such as AAS, TGA and CHNSO analyzer

CHEM 464: ADVANCED ORGANIC CHEMISTRY

1. REACTIVE INTERMEDIATES
• Carboanion: types, production and reactions
• Carbenes and niterenes: types, production and reactions
• Free radicals: types, production and reactions

2. REARRANGEMENT REACTIONS
• Concept and types of rearrangement reactions
• Important Named reactions with mechanism and synthetic applications
• Wagner-Meerwein, pinacol, Demjanov, Tiffeneau-Demjanov, Backman, Benzylic acid, Hoffmann, Curtius, Lossen, Schmidt rearrangements, etc.

3. PERICYCLIC REACTIONS
• Basic concepts and types; a review of molecular orbital theory and delocalization of orbitals
• Conrotatory and disrotatory process, Woodward-Hoffmann rules and their explanation, frontier orbital approach
• Cycloaddition and cycloreversion reactions
• Suprafacial and antarafacial addition; sigmatropic rearrangements; Cope and Claisen rearrangements

4. OXIDATION-REDUCTION REACTIONS

• Concept and various general reactions with mechanism
• Important oxidation reactions and their mechanism, oxidation of alcohols and aldehydes, carbon-carbon double bonds, etc.
• Common oxidizing agents and their applications, Jones, Collins, Corey, etc.
• Reduction reactions: concept and various reactions, reduction with dissolving metals, birch reduction, different hydrogenation reactions
• Common reducing agents and their applications, LiAlH₄, NaBH₄, etc.

CHEM 464: LAB ACTIVITIES

Experiments based on one-and multi-step synthesis; students are trained for independent organic synthesis, recrystallization and percentage yield calculation.

• Preparation of benzopinacol from benzophenone and 2-Propanol
• Preparation of phenyl-aza-beta-naphthol
• Preparation of dibenzalacetone from benzaldehyde and acetone
• Preparation of benzalacetophenone from acetophenone and benzaldehyde
• Preparation of epoxide of benzalacetophenone from benzalacetophenone
• Preparation of benzil from oxidation of benzoin
• Preparation of benzilic acid from benzil using potassium hydroxide and hydrochloric acid
• Preparation of methyl orange indicator
• Preparation of orange II (1-p-sulfobenzeneazo-2-naphthol sodium salt)
• Preparation of benzoic acid by oxidation with KMnO₄
• Oxidative free radical coupling of 2-naphthol with ferric chloride
• Preparation of benzopinacol from benzophenone and 2-Propanol by microwave

CHEM 465: NATURAL PRODUCTS & MEDICINAL CHEMISTRY

1. NATURAL PRODUCTS

• Introduction, definition, diversity and classification
• Structures and names of various classes: terpenoids, steroids, alkaloids, flavonoids, glycosides, etc.

2. REVIEW OF THE METHODS OF STRUCTURAL ELUCIDATION (CHEMICAL AND SPECTROSCOPIC TECHNIQUES)

3. NATURAL PRODUCTS AND MEDICINES

• The application of natural products in drug discovery, Drug design, Lead compounds
• Aromatherapy
• Perfumes; natural and synthetic

4. TERPENOIDS
• Definition and classification
• Chemical method of structural elucidation
• Examples such as myrcene, citral, geraniol
• Interconversion of some common terpenoids
• Total and partial synthesis of some simple terpenoids, e.g. citral, carvone, alpha-pinene
• Biosynthesis of terpenoids and cholesterol

5. ALKALOIDS
• Different definitions and classifications
• Biosynthetic pathways of some common alkaloids e.g. morphine and its derivatives, role of pyrococcal pp in biosynthesis
• Some examples of tropane, quinoline, isoquinoline, pyridine and indole and steroidal alkaloids, their structures and applications
• Total and partial synthesis of some alkaloids such as ephedrine, coniine

6. FLAVONOIDS
• Types of flavonoids such as, flavones, flavans, flavanones, isoflavans, neoflavans etc.
• Synthesis of some flavonoids, flavone, flavonol and cyanidin
• Biosynthesis of Flavonoids: cyanidin and flavone, etc.

7. MEDICINAL IMPORTANCE OF POLYPHENOLS, GLYCOSIDES
• Antioxidant activities and free radical scavenging mechanisms

8. STEROIDS, HORMONES, CHOLESTEROL
• Structure, biosynthesis and applications

CHEM 465: LAB ACTIVITIES

Experiments are arranged based on isolation techniques and structure determination of natural products. Examples:
• Phytochemical screening of phytochemicals (alkaloids, terpenoids, flavonoids, glycosides, tannins etc.) in different plant samples (leaves, bark, flowers, seeds etc.); preparation of related reagents and their applications, such as Meyer, Wagner, Hager, Dragendorff reagents
• Paper chromatography of plant pigments (spray reagents, benedict solution, iodine vapors)
• Isolation of essential oils from cloves using steam distillation
• Isolation of lycopene from tomato
• Isolation of carotenoids from carrot
• Isolation of limonene from orange peel
• Isolation of nicotine from tobacco
• Isolation of caffeine from tea leaves
• Isolation of piperine from black pepper
• Isolation of cinnamaldehyde for cinnamon

CHEM 470: POLYMER CHEMISTRY

1. INTRODUCTION AND CHARACTERIZATION OF POLYMERS
   • Synthetic routes to polymers
   • Molecular weight determination
   • Composition and microstructure
   • Optical microscopy
   • Electron microscopy
   • Analytical microscopy
   • Thermal analysis
   • Molecular relaxation spectroscopy
   • X-ray and neutron scattering methods

2. GENERAL PROCEDURES IN CHAIN-GROWTH POLYMERIZATION
   • Free-radical chain polymerization
   • Anionic polymerization
   • Ring-opening polymerizations initiated by anionic reagents
   • Coordination polymers

3. CONTROLLED/‘LIVING’ POLYMERIZATION METHODS
   • Covalent ‘living’ polymerization
   • Group transfer polymerization
   • Controlled free-radical polymerizations mediated by nitroxides
   • Controlled free-radical polymerizations
   • Atom transfer free-radical polymerizations (ATRP) and aqueous ATRP

4. STEP-GROWTH POLYMERIZATION
   • The synthesis of an aromatic polyamide
   • Preparation of a main-chain liquid crystalline poly(ester ether) with a flexible side-chain
   • Non-periodic crystallization from a side-chain bearing Co-polyester
5. THE SYNTHESIS OF CONDUCTING POLYMERS BASED ON HETEROCYCLIC COMPOUNDS
   - Electrochemical synthesis
   - Synthesis of polypyrrole, polyaniline and polythiophene

6. DENDRIMER SYNTHESIS
   - Excess reagent method
   - Protection–deprotection method.

7. NEW METHODOLOGIES IN THE PREPARATION OF IMPRINTED POLYMERS
   - Sacrificial spacer approach
   - Preparation of bacteria-imprinted polymers

8. LIQUID CRYSTALLINE POLYMERS
   - Synthesis of an acrylate-based liquid crystal polymer
   - The hydrolytic reaction
   - A useful procedure for the preparation of a variety of side-chain polymers
   - Photochemical preparation of liquid crystalline elastomers with a memory of the aligned cholesteric phase
   - Defining permanent memory of macroscopic global alignment

CHEM 470: LAB ACTIVITIES
   - Synthesis of marked free radical, addition and condensation polymers.
   - Understandings of the solution, suspension and colloidal polymerization.
   - Biopolymers: Characterization and Functionalization
   - Development recyclable polymers
   - Polymer Characterization with Help of Analytical Instruments

CHEM 472: ADVANCED QUANTUM CHEMISTRY
   - Angular momentum
   - Approximate methods
   - Perturbation theory, Multielectron atom
   - Molecular orbital calculations
   - Computational quantum chemistry

CHEM 473: SURFACE AND SOLID STATE CHEMISTRY
   - Crystal structures, Unit cells and Miller indices
   - X-ray diffraction
• Adsorption and desorption
• Langmuir and BET isotherms
• Surface reactions and reactivity
• Ultrathin films and interfaces
• Techniques for the study of surfaces

CURRENT RESEARCH PROJECTS

Currently, different research groups comprising faculty members and students are actively engaged in various research activities. The titles of some research projects are given below:

- Phytochemical and biotechnological studies on antioxidant and anti-microbial compounds in Lagenaria siceraria.
- Activity-guided isolation of bioactive chemical constituents from roots of Carissa opaca.
- Metal drug complexation through mechanochemistry and their biological activities.
- Optimizing condition for the preparation of chloro cyanurate.
- Mechanochemical synthesis and characterization of 1st transition metal complexes with Dimethylglyoxime.
- Mechanochemical synthesis and characterization of metal complexes with Dimethylglyoxime.
- Synthesis of zero valent nanoparticles for hydrogen generation.
- Anticancer studies of different plant extracts using Ames test.
- Identification and analysis of heavy metal toxicity in plant samples and their soil sources.
- Antioxidant and antimicrobial activity of Cassia fistula fruits.
- GCMS analysis and anti-microbial activity of methanolic extract and various fractions of Ehretia serrata.
- GCMS analysis and anti-microbial activity of methanolic extract and various fractions of Adiantum caudatum.
- Characterization and identification of drug metabolic from hair samples of addicted persons.
- Synthesis and characterization of silver nanoparticles.
- Synthesis of polymer coated magnetic nanoparticles for drug delivery.
- Study of biocompatible polymers.
- Enzymatic study and antioxidant activity of *Fagonia cretica*.
- Synthesis and characterization of methotrexate drug with transition metals.
- Isolation of Ephedrine from Ephedra by complexation method.
- Reaction of 3-formyl chromone with amino benzene sulfonamide.
- Synthesis, characterization and evaluation of biological activities of transition metal complexes of sulfonamides derived from formyl chromones.
- Synthesis and SAR studies of anti-microbial sulfonamides.
- Synthesis and characterization of potentially active sulfonamides and carboxamide derivatives.
- Transition metal complexes of sulfonamides derived from substituted 3-formyl chromones.
- Synthesis and characterization of transition metal complexes of 4-(2-Aminoethyl) benzolsulfonamide.
- Synthesis and characterization of transition metal complexes of 4-(2-Aminomethyl) benzolsulfonamide.
- Absorption of different dyes on activated carbon.
- Effect of doping on super conductors.
- Isolation of activated ingredients from garlic by complexation method.
- Calorimetric study of carbohydrate polymers.
- Evaluation of polysaccharides for various pharmaceutical applications.
- Study of timolol from arabinosylan gel.
- Inter-conversional thermal analysis of AlCl$_3$.6H$_2$O and FeCl$_3$.6H$_2$O.
- Study of N-Chlorination of sulfa drugs.
- Physicochemical investigation and antioxidant studies of *Nigeela stiva*.
- Evaluation of antioxidant and antimicrobial activity of *Cassia fistula* Linn. (Amaltas).
- Phytochemical and physico chemical studies of dates (*Phoenix dactilifera* L.), Evaluation of antioxidant and enzymatic activities.
- Study of antioxidant activity of *Syzigium cumini* plant and extraction of dyes from *Syzigium cumini* plant.
- Synthesis, characterization and evaluation of biological activity of Seleno-organic compounds.
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On study leave