

Curriculum Chemical Sciences (SC)

Analytical chemistry Organic chemistry Inorganic chemistry Physical chemistry Pharmaceutical science Biotechnology



ANALYTICAL CHEMISTRY (SC)

Data Acquisition and Use of Statistics

- Errors
- Statistical considerations
- Homogeneous and Heterogeneous Equilibria
- Acid-base
- Oxidation-reduction
- Complexometry
- Gravimetric analysis
- Solubility
- Precipitation titrations
- Chemical separations
- Extractions

Instrumental Methods

- Electrochemical methods
- Spectroscopic methods
- Chromatographic methods
- Calibration of instruments



INORGANIC CHEMISTRY (SC)

AtomicStructure

- The Schrödinger Equation
- Atomic orbitals
- Electronic configurations the PeriodicTable
- Periodic Properties of Atoms

Bonding Theory

- Electrostatic interactions (ionic bonding)
- The Lewis theory of covalent bonding
- The valence bond (VB) theory
- The molecular orbital (MO) theory
- Applications of the MO theory to simple biatomic molecules
- The metallic bond
- The hydrogen bond
- Van der Waals forces

Acid–Base and Donor–Acceptor Chemistry

- Arrhenius Concept
- Brønsted–Lowry Concept
- Lewis Acid–Base Concept and Frontier Orbitals
- Acidity in nonaqueous solvents
- The Hammett acidity function Superacids
- Hard and Soft Acids and Bases
- Aqua complexes of metal cations

The Crystalline Solid State

- The hard sphere model: close packings
- The metallic bond: fundamentals of band theory
- Physical and physico-chemical properties of elements in the solid state
- Ionic solids: the electrostatic model
- Lattice energy in ionic solids and its chemical implications

Chemistry of the Main Group Elements

- General Trends in Main Group Chemistry
- Compounds with hydrogen of the main group elements
- Compounds with oxygen of the main group elements
- Compounds with halogens of the main group elements
- General features of the elements of the single main groups
- Diagonal relationships

Chemistry of the Transition Elements

- Periodic Trends within the Transition Elements
- Transition series: similarities and differences

Coordination Chemistry

- Types of ligands, nomenclature and formulas
- Coordination numbers and geometries
- Isomerism
- Crystal Field Theory
- The spectrochemical series
- High- and low-spin complexes
- The Curie law for magnetically diluted spin systems
- Spin-only paramagnetism in transition metal complexes
- Crystal field stabilization energy and its chemical implications
- Complex formation: stability constants
- The Irving-Williams series
- The chelate effect
- Spinel structure
- Hydration enthalpy of 3d metal di-cations
- Lattice energy of 3d metal di- and tri-halides
- Tetragonal distorsion in octahedral complexes



- Square planar complexes of nd8 ions
- Molecular orbital theory in coordination chemistry (octahedral complexes)
- Sigma- and pi-bonding
- Pi-basic and -acid ligands
- The 18-electron rule for complexes of pi-acid ligands
- Electron spectroscopy of metal complexes
- Selection rules
- d-d and CT transitions
- electronic configuration and number of spin-allowed d-d bands
- Substitution reactions in octahedral complexes
- The crystal field activation energy



ORGANIC CHEMISTRY (SC)

- The Structures of Organic Molecules
- Structural components of organic molecules
- Systematic nomenclature: IUPAC names
- Constitutional isomers and hydrocarbon substituents

Bonding in Organic Molecules

- Lewis structures
- Bond properties
- Resonance structures
- Hybrid orbitals and shapes of molecules
- Delocalized $\pi\text{-}electron\ systems$
- Noncovalent interactions

The Conformations of Organic Molecules

- Conformations of acyclic compounds
- Conformations of cyclic compounds
- Conformations of substituted cyclohexanes and cyclic compounds

The Stereochemistry of Organic Molecules

- Geometric isomers of alkenes
- Chirality and enantiomers
- Diastereomers
- Fischer projections

Chemical reactions and mechanisms

- General aspects of reactions
- Acid-base reactions
- Reaction mechanisms
- Reaction coordinate diagrams
- Kinetics of organic reactions
- Kinetic and thermodynamic control on selectivity

Substitution reactions of alkyl halides

- The SN1-reaction and the SN2-reaction of alkyl halides

Substitution reactions of alcohols and related compounds

- Substitution reactions of alcohols
- Substitution reactions of ethers and epoxides
- Substitution reactions of thiols and thioethers

Elimination reactions of alkyl halides, alcohols and related compounds

- The E1-reaction
- The E2-reaction

Addition reactions of alkenes and alkynes

- Electrophilic addition reactions of alkenes
- Electrophilic addition reactions of alkynes
- The formation of carbon-carbon bonds
- Hydroboration reactions of π -bonds
- The addition of carbenes to π -bonds

Addition reactions of conjugates dienes

- The structures of dienes
- Bonding in conjugated dienes
- Electrophilic addition to conjugates dienes

Oxidation and reduction reactions

- Oxidation states in organic molecules
- Hydrogenation reactions
- Oxidation reactions of alkenes
- Oxidation reactions of alcohols
- Oxidation reactions of amines

Free radical reactions

- Free radical halogenation reactions
- Reduction via radical intermediates



- Free radical addition reactions
- Oxidation via radical intermediates

Determining the structures of organic molecules

- 1H and 13C NMR spectroscopy
 - Chemical shifts and proton equivalence
 - Spin coupling
 - Interpreting and predicting 1H NMR spectra
 - Carbon NMR spectra
- Mass spectrometry
- Infrared spectroscopy

Organometallic reagents and chemical synthesis

- Carbon-carbon fond formation
- Organomagnesium and lithium compounds
- Transition metal organometallic compounds

Asymmetric reactions and synthesis

- Chiral compounds
- Enantiomeric resolution
- Asymmetric synthesis

The chemistry of benzene and its derivatives

- Structural aspects of aromatic molecules
- Electrophilic substitution reactions of benzene
- Electrophilic substitution reactions of benzene derivatives
- Nucleophilic substitution reactions of benzene derivatives
- Aromatic diazonium salts

Nucleophilic addition reactions of aldehydes and ketones

- General aspects of nucleophilic addition reactions
- Nucleophilic addition reactions
- Reduction reactions of aldehydes and ketones
- Oxidation reactions of aldehydes and ketones

Addition-substitution reactions of aldehydes and ketones

- Hemiacetals and acetals
- Acetals as protecting groups
- Carbohydrates

Addition-elimination reactions of aldehydes and ketones

- Compounds with carbon-nitrogen double bonds
- Imines, enamines, ylides

Addition-elimination reactions of carboxylic acids and derivatives

- Reactions of carboxylic acids
- The chemistry of acid chlorides, thioesters, and anhydrides
- The chemistry of esters
- The chemistry of amides
- The chemistry of nitriles
- Reactions with organometallic compounds

- Reduction reactions of carboxylic acids and derivatives

The acid-base chemistry of carbonyl compounds

- Acidity of carbonyl compounds
- Enols and enolate ions
- Reactions of enolate ions
- Dicarbonyl compounds

The nucleophilic addition reactions of enolate ions

- The aldol reaction
- The Claisen-condensation

Conjugate addition reactions of unsaturated carbonyl compounds

- α,β-Unsaturated carbonyl compounds
- Conjugate addition reactions
- Conjugate addition reactions of carbanions



The chemistry of polycyclic and heterocyclic arenes

- Polycyclic aromatic compounds
- Pyridine, pyrrole, azoles and related heterocycles
- Amino acids, peptides, and proteins
- Amino acids
- Chemical synthesis of amino acids
- Peptide synthesis and analysis



PHYSICAL CHEMISTRY (SC)

Gases

- The gas laws
- The van der Waals equation
- The principle of corresponding states

The first law of thermodynamics

- Work, heat, and energy
- Internal energy
- Expansion work

State functions

- Exact and inexact differentials
- Changes in internal energy
- The Joule-Thomson effect

Enthalpy and thermochemistry

- Heat exchange and enthalpy
- Standard enthalpy changes
- Temperature-dependence of reaction enthalpies

The second law of thermodynamics

- Entropy, entropy changes accompanying specific processes
- The third law of thermodynamics

Free energy

- The Helmholtz and Gibbs free energies
- Standard reaction Gibbs free energies
- Partial molar quantities
- Chemical potential

Thermodynamics of mixing

- Chemical potential of liquids
- Ideal solutions
- Colligative properties
- Activities in solution

Phases and phase changes

- Phase transitions and phases diagrams
- The phase rule
- Vapor-pressure diagrams
- Temperature-composition diagrams

Thermodynamics of chemical reactions

- Free energy minimum

- Equilibrium
- Effect of pressure on equilibria
- Effect of temperature on equilibria

Electrochemical thermodynamics

- Electrodes and half-reactions
- The electromotive force and its relation to the Gibbs free energy
- Nernst equation
- Standard potentials

- Applications of standard potentials

Quantum mechanics

- Wave-particle duality
- The Schrödinger equation
- The uncertainty principle
- The postulates of quantum mechanics

Quantization of motion

- Particle in a box
- Tunneling
- Vibrational motion



- Rotation in two and three dimensions
- Spin
- Time-independent perturbation theory
- Time-dependent perturbation theory

Atomic orbitals

- The structure of hydrogenic atoms
- Atomic orbitals and their energies
- Spectroscopic transitions and selection rules
- The structures of multielectron atoms
- The orbital approximation
- Self-consistent field orbitals

Electronic transitions

- The spectra of complex atoms
- Singlet and triplet states
- Spin-orbit coupling
- Term symbols and selection rules

Molecular orbitals

- The Born–Oppenheimer approximation
- Molecular orbital theory
- The hydrogen molecule ion
- Homo- and heteronuclear diatomic molecules
- Molecular orbitals for polyatomic systems
- The Hückel approximation
- Prediction of molecular properties
- Symmetry elements
- Selection rules

Electric properties of molecules

- Electric dipole moments
- Polarizabilities

Molecular spectroscopy

- Absorption and emission spectroscopies
- The intensities of spectral lines
- Molecular vibrations
- Anharmonicity
- Vibrations of polyatomic molecules
- Franck-Condon principle
- Normal modes
- Infrared absorption spectra of polyatomic molecules
- Symmetry aspects of molecular vibrations
- The electronic spectra of diatomic molecules
- The electronic spectra of polyatomic molecules
- Fluorescence and phosphorescence
- Dissociation and predissociation

Magnetic spectroscopy

- Energy of electrons in magnetic fields
- Energy of nuclei in magnetic fields
- Magnetic resonance spectroscopy
- Chemical shift
- Fine structure
- Electron paramagnetic resonance
- Hyperfine structure

Statistical thermodynamics

- The Boltzman distribution
- The molecular partition function
- The canonical ensemble
- Internal energy and entropy



Chemical kinetics

- Fundamentals of chemical kinetics
- Experimental techniques
- Reaction rate
- Integrated rate laws
- Temperature dependence of the reaction rates
- Collision and transition-state theories
- Principles of homogeneous catalysis
- Enzymatic reactions
- The rates of electron-transfer reactions
- The theory of electron transfer



PHARMACEUTICAL SCIENCE (SC)

Physical, chemical and pharmaceutical properties of drugs

Drug design:

hit discovery strategies, hit to lead optimization strategies, combinatorial chemistry, structure-based and mechanismbased design methods;

General concepts on pharmacokinetics and pharmacodynamics:

drug absorption, distribution, elimination and metabolism (phase I and phase II reactions).

Drug targets and target recognition:

proteins, enzymes, receptors and nucleic acids as targets, mechanisms of inhibition

Biodrugs

PREFORMULATION

- Background in physical pharmaceutics and biopharmaceutics.
- Dissolution and solubility, physical state, contact angle, polymorphism, micro and nano-nization, solid solutions.
- Diffusion, Fick's laws, Higuchi's law, semiempirical laws.

MICROMETRICS

- Calorimetry, DSC, DTA, TGA
- Particle size: methods and data analysis

-Surface area, porosity, powder density and flow

- -Mechanical properties: elasticity and plasticity
- Principles of rheology

DOSAGE FORM CHARACTERIZATION

- Knowledge of main physicochemical and biopharmaceutical properties of major classes of pharmaceutical structural excipients, namely polymers, lipids, surfactants, sugars etc

- Knowledge of classical analytical techniques for physicochemical and biopharmaceutical characterization of biomaterials and products for drug administartion.

ADVANCED DRUG DELIVERY SYSTEMS and NANOTECHNOLOGY

- Dispersed systems: suspensions and emulsions
- Polymeric and inorganic microparticles
- Colloidal systems polymeric nanoparticles, inorganic nanoparticles, liposomes, micelles, polymersomes, physical assemblies, polymer bioconjugates, solid lipid nanoparticles.
- Cyclodextrins
- Hydrogels
- Principles of drug targeting



BIOTECHNOLOGY (SC)

MOLECULAR BIOLOGY

Nucleic acid structure DNA replication Transcription in Prokaryotes and Eukaryotes RNA maturation Translation Most important techniques: electrophoresis, blotting, cloning, polymerase chain reaction (PCR)

BIOCHEMISTRY

Structures and properties of amino acids and proteins Protein folding and post-translational modifications Protein-protein interaction Cooperativity and allostery in macromolecules Catalysis and enzyme kinetic Structure and properties of lipids and membranes Molecular mechanisms of signal transduction Glycolysis, Krebs cycle, oxidative phosphorylation

MICROBIOLOGY

Structural and metabolic properties/characteristics of prokaryotic and eukaryotic microorganisms Microbial growth Relevant industrial fermentation processes

GENETIC ENGINEERING

Recombinant DNA technologies Production of heterologous proteins Main techniques for the isolation and characterization of proteins and peptides DNA sequencing

BIOINFORMATICS

Databases of interests to Biotechnologies and data mining Tools to retrieve, analyze and compare protein and nucleic acid sequences Consensus sequences, functional motifs and profiles Protein structure comparison and modelling

"OMIC" SCIENCES

Isolation and purification of genomic DNA DNA genomic libraries Genetics and Physics mapping of a genome Basic concepts of Transcriptomics and Proteomics



Curriculum Pharmaceutical Sciences (SF)

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- Acetals as protecting groups
- Carbohydrates

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- Reactions of carboxylic acids
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- The chemistry of esters
- The chemistry of amides
- The chemistry of nitriles
- Reactions with organometallic compounds

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- Reactions of enolate ions
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- The aldol reaction
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- α,β-Unsaturated carbonyl compounds
- Conjugate addition reactions
- Conjugate addition reactions of carbanions



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- Polycyclic aromatic compounds
- Pyridine, pyrrole, azoles and related heterocycles
- Amino acids, peptides, and proteins
- Amino acids
- Chemical synthesis of amino acids
- Peptide synthesis and analysis



GENERAL CHEMISTRY (SF, Inorganic+Physical chemistry)

Inorganic Chemistry

Atoms and electronic configuration Chemical compounds Chemical bonding Solutions and Their Physical Properties Solutions and colligative properties Chemical reactions State diagrams Principles of Chemical Equilibrium Equilibria in solution: solubility, pH, complex formation Electrochemistry Equilibria in the gas phase Periodic Table and Some Atomic Properties Coordination compounds

Physical Chemistry

Classical thermodynamics: basic definitions

- Open, closed, isolated systems
- State of a system and state functions

The first law of thermodynamics

- Work, heat, internal energy and the formulation of the first law

Enthalpy and thermochemistry

- Heat exchange and enthalpy
- Standard reaction enthalpy
- Temperature-dependence of reaction enthalpies

The second law of thermodynamics

- Entropy and the formulation of the second law
- The third law of thermodynamics

Free energy

- The Gibbs free energies
- Standard reaction Gibbs free energies
- Partial molar quantities
- Chemical potential

Thermodynamics of mixing

- Ideal solutions
- Colligative properties
- Activities in solution

Phases and phase changes

- Phase transitions and phases diagrams

Thermodynamics of chemical reactions

- Free energy minimum
- Thermodynamic equilibrium constant and standard reaction free energy
- Effect of temperature on equilibria: van't Hoff equation

Electrochemical thermodynamics

- Electrodes and half-reactions

- The electromotive force and its relation to the Gibbs free energy
- Nernst equation
- Standard potentials

Quantum mechanics

- Wave-particle duality
- The Schrödinger equation
- The uncertainty principle
- **Atomic orbitals**



- The structure of hydrogenic atoms
- Atomic orbitals and their energies
- The structures of multielectron atoms

Molecular orbitals

- The Born–Oppenheimer approximation
- Molecular orbital theory
- Homo- and heteronuclear diatomic molecules
- Molecular orbitals for polyatomic systems

Molecular spectroscopy

- Absorption and emission spectroscopies
- Molecular vibrations
- Vibrations of polyatomic molecules: Normal modes
- Infrared absorption spectra of polyatomic molecules
- The electronic spectra of molecules
- Fluorescence and phosphorescence

Chemical kinetics

- Reaction rate and rate law
- Integrated rate laws
- Temperature dependence of the reaction rates
- Enzymatic reactions: Michaelis-Menten kinetics



PHARMACEUTICAL CHEMISTRY (SF)

PRINCIPLES OF MEDICINAL CHEMISTRY

Physical, chemical and pharmaceutical properties of drugs

Drug design: hit discovery strategies, hit to lead optimization strategies

Combinatorial chemistry

General concepts on pharmacokinetics and pharmacodynamics: drug absorption, distribution, elimination and metabolism (phase I and phase II reactions). Proteins, enzymes, receptors and nucleic acids as targets, mechanisms of inhibition

MECHANISMS OF DRUG ACTION AND STRUCTURE-ACTIVITY RELATIONSHIPS

Antibiotics and Antimicrobial agents

Cell wall synthesis inhibitors, Bacterial protein synthesis inhibitors, DNA gyrase inhibitors

Antifungal agents

Antimycobacterial Agents Antitubercolin drugs – Antileprotics

Antiparasitic Agents

Antimalarials- Anthelmintics – Amoebicides- Antiprotozoals

Antiviral agents

Neuraminidase inhibitors, Entry inhibitors, Agents interfering with viral nucleic acid replication. Nucleoside Reverse Transcriptase inhibitors, Protease inhibitors, Integrase inhibitors.

Antineoplastic drugs

Drugs that react with nucleic acids, Topoisomerase-directed drugs, Antimetabolites, Mitosis inhibitors, Kinases inhibitors, Therapeutic strategies for hormone-dependent cancers, Novel anticancer approaches.

Anti-inflammatory drugs

Nonsteroidal anti-inflammatory drugs Steroidal anti-inflammatory drugs

Drugs for the Cardiovascular System

Cardiac agents -Antihypertensive drugs- Antihrombotics drugs-Antihyperlipoproteinemics and inhibitors of choles-terol

Drugs Affecting the Central Nervous System

Drugs used to treat neuromuscular disorders -Sedative-Hypnotics -Anxiolytic drugs -Antipsychotic drugs - Antiseizure drugs - Antidepressants -Hallucinogens and Central stimulants - Central Analgesics. General Anesthetics. Local Anesthetics

Drugs Affecting the Histaminergic System

H₁ Antihistamines, H₂ Antihistamines, Proton pomp inhibitors

Drugs Affecting Cholinergic Neurotransmission

Muscarinic Agonists, Acetylcholinesterase Inhibitors, muscarinic antagonists, nicotinic antagonists

Hormons in therapy.



PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY (SF)

PREFORMULATION CONCEPTS

- Background in physical pharmaceutics and biopharmaceutics.

Bioavailability, BCS

-Route of administration

- Basic principles dictating the selection and the design of dosage forms: traditional dosage forms and micro- and nano-pharmaceuticals.

BIOPHARMACEUTICAL FEATURES OF DOSAGE FORMS

- Drug absorption: mechanisms and pathways. Membrane transport mechanisms: Passive, active, facilitated, pinocy-tosis, ion-pairing. Influx and efflux pumps, paracellular and transcellular pathways.

-Principles of pharmacokinetics: non compartmental and compartmental analyses. Mono-compartmental model with and without absorption step, bi-compartmental model with and without absorption step, pharmacokinetic parameter analysis.

- Dissolution and solubility, physical state, contact angle, polymorphism, micro and nano-nization, solid solutions.

- Diffusion, Fick's laws, Higuchi's law, semiempirical laws.

-Biopharmaceutical performance of solubilizers, stabilizers, targeting agents, cell penetrating enhancers, mucoadhesive materials, stimuli sensitive materials.

MICROMETRICS

- Familiarity with classical analytical techniques for physicochemical and biopharmaceutical characterization of ingredients and dosage forms.

- Calorimetry, DSC, DTA, TGA
- Particle size: methods and data analysis
- -Surface area, porosity, powder density and flow
- -Mechanical properties: elasticity and plasticity

- Principles of rheology

- Knowledge of main physicochemical and biopharmaceutical properties of major classes of structural excipients (natural and synthetic polymers, lipids, surfactants, polysaccharides, etc.)

DOSAGE FORMS AND THEIR FORMULATION PROCESS

- Current methodologies in preparation of conventional pharmaceutical dosage forms and advanced formulations.

- Solid forms: tablets and capsules
- Inhalables: nasal, bronchial and pulmnonary delivery
- Topical systems
- Injectables and sterilization, lyophilization.
- Hydrogels

- Main processes of pharmaceutical technology: mixing and blending, milling, desiccation, spray drying, granulation, tableting, coating.

ADVANCED DRUG DELIVERY SYSTEMS and NANOTECHNOLOGY

- Knowledge of principles of controlled drug delivery and drug targeting.
- Two-phase dispersed systems: suspensions and emulsions.

- Colloidal systems: polymeric nanoparticles, inorganic nanoparticles, liposomes, micelles, polymersomes, physical assemblies, polymer bioconjugates, solid lipid nanoparticles.

- Cyclodextrins and their use as excipients.
- Responsive formulations, stimuli-sensitive drug delivery systems.
- Principles of drug targeting.



BIOTECHNOLOGY (SF)

MOLECULAR BIOLOGY

Nucleic acid structure DNA replication Transcription in Prokaryotes and Eukaryotes RNA maturation Translation Most important techniques: electrophoresis, blotting, cloning, polymerase chain reaction (PCR)

BIOCHEMISTRY

Structures and properties of amino acids and proteins Protein folding and post-translational modifications Protein-protein interaction Cooperativity and allostery in macromolecules Catalysis and enzyme kinetic Structure and properties of lipids and membranes Molecular mechanisms of signal transduction Glycolysis, Krebs cycle, oxidative phosphorylation

MICROBIOLOGY

Structural and metabolic properties/characteristics of prokaryotic and eukaryotic microorganisms Microbial growth Relevant industrial fermentation processes

GENETIC ENGINEERING

Recombinant DNA technologies Production of heterologous proteins Main techniques for the isolation and characterization of proteins and peptides DNA sequencing

BIOINFORMATICS

Databases of interests to Biotechnologies and data mining Tools to retrieve, analyze and compare protein and nucleic acid sequences Consensus sequences, functional motifs and profiles Protein structure comparison and modelling

"OMIC" SCIENCES

Isolation and purification of genomic DNA DNA genomic libraries Genetics and Physics mapping of a genome Basic concepts of Transcriptomics and Proteomics