



COURSE DESCRIPTIONS

Bachelor's Degree in Chemistry

➤ **1st year**

5263 MECHANICS AND THERODYNAMICS

Unit 1. Magnitudes, units and dimensional analysis

Fundamental characteristics of physical systems. Domains of physics. Magnitudes and measures. Unit systems and dimensional equations. Système International d'Unités (S.I.). Error theory. Vectors and vector algebra.

Unit 2. Kinematic and dynamic

Reference systems and coordinate systems. Particle kinematics. Movement of a particle system. Relativity of the movement. Inertial and non-inertial systems. Interactions and forces. Newton's laws. Balance of a Particle. Friction forces. Central forces. Consideration of Newton's Laws applied to problem solving. Work and energy. Potential energy. Conservation of the mechanical energy of a particle. Potential diagram.

Unit 3. Particle systems. Conservation theorems

Introduction. external and internal forces. Differential equations of the movement of a particle system. First movement equation. Center of Mass and Properties. Linear moment: Principle of conservation. Angular momentum. Second equation of motion. Principle of conservation of angular momentum. Conservation of mechanical energy for a particle system.

Unit 4. Rotation dynamics

Kinematics of rotation. Kinetic energy of rotation. Calculating moments of inertia. Kinematics of the rigid body. Rigid body dynamics. Analogy between kinematic and dynamic variables in translation and rotation. Angular momentum of a rigid solid: its conservation. Applications.

Unit 5. Gravitation

Kepler's laws. Newton's law of universal gravitation. Gravitational mass and inertial mass. Gravitational potential energy and orbital motion. The gravitational field.

Unit 6. Fluid static. Hydrodynamics

Density. Pressure in a resting fluid. Archimedes' principle. Dynamics of Fluids. Continuity equation. Bernoulli's equation; Applications. Real fluids. Viscosity...

5264 MATHEMATICS (I)

Study of functional models dependent on one and on several variables.

Domain definition properties.

Basic topology (open, closed, narrowed, compact, connected).

Operations with functions, regularity properties and optimization

Continuity, derivability, differentiation, extremes and conditional extremes.

Integral

Primitive. Defined Integral. Fundamental theorems of integral calculus. Calculation of integrals.

Basic Models

Polynomial models, exponential, logarithmic, trigonometric. Models of Growth and degrowth.

Chemical process models. Interpretation. Optimization.

Functional approximation

Polynomial local approximation: Taylor expressions. Error evaluation of the approximation.

Numerical approximation

Methods of discretization and iterative methods.

Approximation techniques for models of one variable: root search, numerical squaring.

5265 GENERAL CHEMISTRY (I)

Unit 1: Atomic structure

Topic 1.1.-Inorganic formulation and nomenclature.

Elements and isotopes. Binary compounds: oxides and hydrides. Oxyacids and Oxyalts. Acid salts. Basic salts. Double salts. Adducts. Complexes. Principle of generalized coordination.

Topic 1.2.-Historical evolution. Wave mechanics.

Historical evolution of the concepts of the structure of matter. Experimental bases for the present-day atomic model: the new phenomena. Wave mechanics. Wave function and its meaning: wave equations. Particle in a box model (infinite potential well).

Topic 1.3.-The hydrogen atom.

Schrödinger equation applications. Hydrogen-like atomic orbital. Wave function study. Radial function and angular function. Quantum numbers. Probability functions. Electronic density maps.

Topic 1.4.-Polyelectronic atoms.

Electronic configuration. Shielding and effective nuclear charge. Spin function. Periodic table. Periodic properties: atomic radius, ionization potential, electronic affinity, electronegativity.

Unit 2: Molecular bond and structure (I).

Topic 2.1.-Bonding theories.

Molecular orbital theory. Valencia liaison theory. Orbital hybridization. Resonance.

Topic 2.2.-Diatomic molecules.

Application to homonuclear and heteronuclear diatomic molecules. Electronic configuration. Bond order. Bond polarity and electronegativity.

Topic 2.3.-Polyatomic molecules.

T.O.M.: Correlation Diagrams. Lewis structures. Model of repulsion between pairs of electrons from the valence layer. Stereochemistry and molecular geometry. Isoelectronic compounds. Molecular properties.

Unit 3: The bond in condensed phases

Topic 3.1.-The condensed phases.

Solid types: Covalent solids, Metallic solids, Ionic solids, Molecular solids. Analogies and differences. Crystalline nets: unit cell. Compact packaging. tetrahedral and octahedral voids. Reticular defects.

Topic 3.2.-Covalent solids.

Structures of covalent crystals. Structures based on tetrahedral networks. Structures based on octahedral networks.

Topic 3.3.-Metallic solids.

Metals. Crystalline packing of metals. Alloys. Alloy structure. Order-disorder transitions. The metallic bond. Band theory. Permitted bands, forbidden bands. Conductors, insulators and semiconductors.

Topic 3.4.-Ionic solids.

Introduction. Ionic crystal structures. Types of networks: cations occupying octahedral gaps, cations occupying tetrahedral gaps. Relations between ratios. The ionic bond. Reticular energy. Ion pair energy. Ion network energy: Born-Landée equation. Kapustinskii equation. Born-Haber Cycle. Properties of ionic compounds. Polarization, a partial covalent character of the ionic bond, impact on properties.

Topic 3.5.-Molecular solids.

Intermolecular forces. Van der Waals forces. Hydrogen bond. Structure of molecular solids.

Topic 3.6.-Relationship between structure and properties.

Effects of chemical forces. Melting and boiling points. Mechanical properties: hardness and fragility. Solubility. Stability.

Unit 4: Basic concepts of chemical reactivity (I)

Topic 4.1.-Acid-base concepts.



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Definitions of Arrhenius, Brønsted-Lowry, Lux-Flood and Lewis. Hard and soft acids and bases (Pearson classification). Acid-base strength measurement. Variation of acidity/basicity in the Periodic table: basic and acid oxides, basicity of the hydroxides, acidity of the oxoacids. Hydrolysis. Acid-base reactions in solvents
Non-aqueous: NH_3 , H_2SO_4 , BrF_3 .

Topic 4.2.-Oxidation and reduction reactions.

Basic concepts. Semi-reactions. Ionic reaction/molecular reaction. Disproportion and proportion.

Unit 5: Introduction to organic compounds

Topic 5.1. Organic chemistry. Background and historical perspective.

Concept of Organic Chemistry: historical evolution. Nature, sources and origin of organic compounds. Organic products for consumption, social impact of Organic Chemistry.

Topic 5.2. Characteristics and identification of organic compounds.

Characteristics of carbon compounds. Introduction to the techniques of isolation and purification. Determination of the empirical and molecular formula. Structural theory. Isomerism concept. Determination of the structural formula through chemical and spectroscopic methods.

Unit 6: Molecular bond and structure (II)

Topic 6.1. The bond in carbon compounds.

Practical analysis of hybridization and study of the geometry of some simple molecules (methane and ethane; ethylene; acetylene). Comparative application of Frontier Molecular Orbital (FMO) theory to ethane and ethene.

Topic 6.2. Electronic structure of organic molecules.

Practical implications of the concept of electronegativity (polarity of organic bonds). Electronic effects (the inductive effect). Application of the concepts of resonance and resonance energy to simple organic molecules (the conjugative effect). Molecular orbital theory applied to simple organic molecules. Prediction of boiling points, solubility and miscibility through the analysis of weak interactions.

Topic 6.3. Aromaticity.

Introduction. Concept of aromaticity, the rule of Hückel. Aromatic systems with six electrons pi (benzene, heterocycles, aromaticity in carbanions and carbocations). Aromatic systems with two pi electrons. Aromaticity in annulenes. Aromaticity of conjugated polycyclic compounds.

Topic 6.4. Classification and nomenclature of organic compounds.

Classification of organic compounds. Functional Group Concept and homologous series. Hydrocarbons, classification and nomenclature. Nomenclature, classification and structure of the main functional groups. Polyfunctional compounds.

Topic 6.5. Isomerism of organic compounds.

Concept and classification. Constitutional isomerism. Stereoisomerism. Concept of conformation: Rotation around the sigma link. Cis-trans isomerism with respect to double bonds.

Topic 6.6. Chirality and optical activity in carbon compounds.

Analysis of the concept of chirality applied to the study of simple enantiomers.
Properties of enantiomers (polarized light and optical activity).
Absolute configuration of stereogenic centers. Representations on the plane (Fischer projection). Diastereomerism. Enantiomers in alicyclic compounds. Optical activity in compounds without stereocenters.

Unit 7: Basic concepts of chemical reactivity (II)

Topic 7.1. Organic compounds such as acids and bases.

Organic reactions, general considerations. Organic compounds such as acids and bases.
Relationship of chemical structure to acidity and basicity.

5266 BASIC LABORATORY OPERATIONS

BLOCK I: MOODLE PLATAFORM. BASES FOR SCIENTIFIC COMMUNICATION. PREPARATION OF REPORTS AND SPOKEN PRESENTATIONS

TOPIC 1: Introduction to the use of the Moodle virtual platform.

Brief introduction and important features of the platform. How to access the virtual classroom. Basic platform functionality.

TOPIC 2: Preparation of reports and oral presentations on the basis of certain criteria.

BLOCK II: DOCUMENTARY TECHNIQUES. SOURCES OF INFORMATION IN CHEMISTRY

TOPIC 3: Information on the library website.

Services offered through the Web: My user account, electronic forms, Off-Campus. Ubucat: Search for information and exportation of results. Recommended bibliography. Electronic resources acquired by the library. Free Internet Resources selected by the library.

TOPIC 4: Search and retrieval of information.

Indexing. Thesaurus. Boolean operators. Search parameters. Search methodology. User profile. Alerts. RSS feeds.

TOPIC 5: Selection of information resources.

Resources acquired by the library/free resources on the Internet. General resources/Specialized resources. Sources of reference information/sources of full-text information.

TOPIC 6: Specialized information sources for the qualification.

Information resources acquired by the library: databases and journals
Electronic. Resources on the Internet. Open Access.

TOPIC 7: Presentation of an academic study.

Information ethics. Regulations related to bibliographic citations. Differences in different types of appointments. Bibliography citations: Books, book parts, magazines, magazine articles, electronic resources.



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Block III: Safety in the Chemistry Laboratory

TOPIC 8: General risk-prevention concepts in a chemistry laboratory.

Chemical products as risk factors. Chemical product labelling. Security data Sheets. REACH regulation.

TOPIC 9: Design, installations and control elements in laboratories.

Importance in the prevention of the design and distribution of laboratories. Risks of the facilities. Control elements.

5267 ELECTROMAGNETISM, QUANTUM PHYSICS AND OPTICS

Block I. Electromagnetism

TOPIC 1. The electric field.

Electric charge. Coulomb's law. Force exerted by a system of charges. Electric field. Lines of force in the electric field. Conductors and insulators. Applications: movement of charges in electric fields. Electric dipole. Field calculations. Electrical distribution of continuous charges in Coulomb's law. Gauss's law. Calculation of electrical fields. Applications of Gauss's Law.

TOPIC 2. Electric potential energy.

Potential difference. Potential of a system of specific charges. Determination of the electrical field from the potential. Calculating the potential for continuous distribution of charges. Equipotential surfaces. Electrostatic potential energy. Capacity. Capacitors. Storage of electrical energy. Dielectrics. Molecular structure of dielectrics.

TOPIC 3. Electrical circuits.

Electric current. Resistance and OHM's law. Joule's law. Batteries and electromotive force. Electrical circuits: combination of resistances. Kirchhoff rules. Instruments of measurement. Loading and unloading a capacitor.

TOPIC 4. Magnetic field.

Force exerted by a magnetic field on a specific charge. Force exerted by a magnetic field on a circuit. Effect of a magnetic field on whorls and magnets. Magnetic dipole. Magnetic field created by specific charges in movement. Magnetic field created by electrical currents: Law of Biot and Savart. Ampère's Law. Magnetic materials.

TOPIC 5. Movement of charges in magnetic fields.

Movement of a charge in a magnetic field. Applications: Frequency of cyclotron, Mass spectrometer, Thomson E/M experiment, Selector of speeds, Cyclotron, Hall effect.

5268 MATHEMATICS (II)

1. Dynamic Models

Dynamic models: The processes of change in science.

- Dynamics and dynamic systems.
- Ordinary differential equations.
- Introduction to balance and system dynamics.



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- Models of change: kinetics, balance.
- Models for chemical reactions.

2. Linear models

Linear models and linearization: model simplification methods.

- Linear models.
- Matrices and linear systems.
- Vector spaces and transformations.
- Vectors and eigenvalues.
- Matrix Diagonalization.

3. Stochastic Models

Stochastic models: Experimental variability in chemistry.

- Introduction to descriptive statistics.
- Probabilistic models.
- Hypothesis testing and estimation.
- Precision and accuracy
- Introduction to univariate regression. Application to univariate calibration models.

5269 GENERAL CHEMISTRY (II)

Part 1: CHEMICAL THERMODYNAMICS.

TOPIC 0: Practices.

Practices carried out in the area of physical chemistry.

TOPIC 1. Fundamentals of chemical thermodynamics: Enthalpy.

Enthalpy: heat transfer at a constant pressure. Calorific capacities at a constant volume and pressure. Enthalpy variations in changes of state. Enthalpy of reaction: Types. The relationship between enthalpy and internal energy. Standard enthalpy reactions. Hess's law. Variation of the enthalpy of reaction with temperature.

TOPIC 2. Fundamentals of chemical thermodynamics: entropy.

Spontaneous processes and entropy. Entropy variation in systems. Standard entropy reactions. Equilibrium. Gibbs free energy (Gibbs function). Free reaction energy. The effect of temperature.

TOPIC 3. Thermodynamics of gaseous states.

The nature of the gases. Pressure. Alternative pressure units. Gas laws: Boyle's law. Charles' law. Avogadro law. The law of ideal gases. Uses of the law of ideal gases. Gas density. The stoichiometry of the reactants gases. Gas mixes. Real Gases: Deviations of Ideality. Equation of state of the real gases.

TOPIC 4. Thermodynamics of condensed media.

Volatility and intermolecular forces. Variation of vapor pressure with temperature. Boiling, melting and solidification. Phase diagrams. Solubility: molecular nature of the dissolutions. Temperature and solubility. Pressure and gas solubility: Henry's Law. Colligative properties: fall in vapor pressure: Raoult's law. Increase in the boiling point and lowering of the freezing point. Osmosis. Binary liquid mixtures: vapor pressure. Distillation. Azeotropes.

TOPIC 5: Thermodynamics of chemical equilibrium.

Reactions in equilibrium: reversibility of the reactions. Equilibrium and law of action of masses. Thermodynamic origin of equilibrium constants. Equilibrium constants: The equilibrium constant in terms of molar concentrations of gases. Alternative forms of equilibrium constant. The response of equilibrium to changing conditions: Le Châtelier principle.

5270 BIOLOGY

UNIT I: INTRODUCTION TO BIOLOGY

TOPIC 1. Biology concept.

1. Definition of biology. 2. Classification of biological sciences. 3. Levels of organization of living organisms. 4. Organization and classification of living organisms. 5. Evolution of living organisms.

UNIT II. BIOMOLECULES

TOPIC 2. Elemental composition of living matter.

1. Biomolecules and bioelements. 2. Molecular hierarchy in cells. 3. Water. Biological importance and properties.

TOPIC 3. Carbohydrates.

1. Classification and biological function. 2. Biological importance of carbohydrates.

TOPIC 4. Lipids.

1. Concept, classification and biological interest. 2. Fatty acids. 3. Triacylglycerides. 4. Waxes. 5. Phospholipids. 6. Glycolipids. 7. Sterols. 8. Terpenes. 9. Eicosanoids. 10. Carotenoids and other compounds

TOPIC 5. Proteins.

1. Classification and biological function. 2. Amino acids. Peptide link. 3. Levels of organization of proteins. 4. Structure and function ratio.

TOPIC 6. Nucleic Acids.

1. Classification and biological function. 2. Nucleosides and nucleotides. 3. Structure and deoxyribonucleic acid organization. 4. Structure, organization and types of ribonucleic acid. RNA maturation.

TOPIC 7. Vitamins.

1. General considerations. 2. Classification. 3. Nicotinic acid. 4. Riboflavin. 5. Pantothenic acid. 6. Folic acid. 7. Biotin. 8. Thiamine. 9. Pyridoxine. 10. Vitamin B12. 11. Ascorbic acid. 12. Vitamin A. 13. Vitamin D. 14. Vitamin E. 15. Vitamin K.



UNIT III. CELLULAR ORGANIZATION

TOPIC 8. Introduction to the cell.

1. Cell theory. 2. Structures and characteristics of prokaryotes and eukaryotic cells. 3. Structure of eukaryotic cells. 4. Visualization of the cellular architecture. 5. Cell cultures

TOPIC 9. Plasma membrane and the cell surface.

1. Composition and architecture of membranes. 2. Dynamics and fluidity of the Membrane 3. Membrane transport function. 4. Cell surface. 5. Intercellular interactions. 6. Cell wall.

TOPIC 10. The cytoplasm.

1. The cytoplasm. Structure and function of the cytoplasm. 2. The cytoskeleton. Microfilaments, intermediate filaments and microtubules.

TOPIC 11. The ribosomes and the smooth and rugged endoplasmic reticulum.

1. Ribosomes. Structure, composition and physiological function. 2. Endoplasmic reticulum. Structure and chemical composition of membrane and cavities and physiological function.

TOPIC 12. The Golgi complex, the Lysosomes, the Peroxisomes, the Glyoxysomes, and the Vacuole.

1. Structure and function of the Golgi complex. 2. Structure and function of the Lysosomes. 3. Peroxisome structure and function. 4. Structure and function of the Glyoxysomes. 5. Vacuole structure and function 6. Vesicular transit, secretion and endocytosis.

TOPIC 13. Mitochondria and chloroplasts.

1. Structure and chemical composition of the membranes and mitochondrial matrix. 2. Physiological functions of the mitochondria. 3. Structure and chemical composition of the chloroplasts 4. Sheath and thylakoid membranes, intermembrane spaces and stroma. 5. Physiological functions of the chloroplasts.

TOPIC 14. The nucleus.

1. Nuclear structure: nuclear envelope, nucleolus and chromatin. 2. Chromosomes. Number of chromosomes: haploid and diploid character. Centromeres and telomeres.

TOPIC 15. Cell reproduction.

1. The cell cycle. 2. Cell division: Mitosis and meiosis 3. Biological cycles. 4. Regulation of the cell cycle. Cell proliferation and death, apoptosis.

TOPIC 16. The genome.

1. Concept of the gene 2. The genome. 3. Genotype, phenotype, dominance. 4. Research into the human genome.

UNIT IV. BIOLOGY AND SOCIETY

TOPIC 17. Social impact of biology.

1. Biotechnology.
2. Immunology.
3. Biodiversity.
4. Environment.
5. Agriculture and livestock.

➤ 2nd year

5271 ORGANIC CHEMISTRY (I)

Topic 1: General aspects of organic reactions.

General aspects. Kinetic and thermodynamic factors: energy profiles and states of transition. Reaction mechanisms. Reactions in one or several stages: intermediates of reaction. Relationship between structure and reactivity: Hammond postulate. Competitive reactions: kinetic control and thermodynamic control. Types of organic reactions. Intermediate species in organic reactions.

Topic 2: Nucleophilic substitution reactions over saturated carbon

General aspects, possibilities and mechanisms. Factors affecting substitution reactions. Stereochemistry of nucleophilic substitution reactions. Competitive reactions. Reactions of synthetic interest: interconversion of functional groups and formation of new carbon-carbon bonds.

Topic 3: Elimination reactions

General aspects and possibilities. Beta-elimination reactions: mechanisms. Beta-elimination regiochemistry: rules of Saytzeff and of Hofmann. Stereochemistry of beta-elimination processes. Substitution and elimination in competition. Reactions of synthetic interest: synthesis of alkenes and alkynes. Alpha-elimination reactions.

Topic 4: Electrophilic addition reactions

General aspects, possibilities and mechanisms. Factors affecting electrophilic addition reactions. Stereochemistry and regiochemistry of the addition electrophilic reactions. Reactions of synthetic interest: addition reactions to alkenes and alkynes.

Topic 5: Substitution reactions on aromatic systems

Aromatic nucleophilic substitution reactions: general aspects. Mechanisms of aromatic nucleophilic substitution. Reactions of synthetic interest. Aromatic electrophilic substitution reactions: general aspects and reaction mechanism. Factors affecting aromatic electrophilic substitution reactions. Electrophilic substitution reactions in polycyclic aromatic systems. Reactions of aromatic heterocyclic compounds. Reactions of synthetic interest.

Topic 6: Structural determination I. Application of ultraviolet-visible spectroscopy, infrared spectroscopy and mass spectrometry in Organic Chemistry.



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Infrared spectroscopy: frequency group characteristics and distribution of absorption bands. IR spectra of families of organic compounds. Ultraviolet-Visible spectroscopy: selected chromophores, absorption characteristics and correlation tables. Mass spectrometry: methods of Ionization. Electron ionization and ion classes. The molecular ion and molecular formula. EM of hydrocarbons and of compounds with carbon-heteroatomic bonds: fragmentation models.

5272 ANALYTIC CHEMISTRY

Theoretical classes

Topic 1. Concept and method of analytical chemistry.

History of analytical chemistry.

Scientific method applied to chemical analysis.

Stages of the analytical method.

Topic 2. Sampling and preparation and preservation of samples.

Sampling techniques.

Preparation of liquid samples.

Preparation of solid samples.

Topic 3. Quantitative Analysis: Gravimetric methods.

Gravimetric analysis.

Electrogravimetric analysis.

Topic 4. Quantitative Analysis: Volumetric methods.

Fundamentals of volumetric analysis.

Volumetric acid base.

Volumetric formation of complexes.

Redox volumetry.

Volumetric precipitation.

Topic 5. Measurement in analytical chemistry.

Basics.

Quality parameters of an analytical method.

Topic 6. Fundamentals of qualitative analysis.

Types of reagents and useful reactions in qualitative analysis.

Systematic qualitative analysis.

Topic 7. Fundamentals of instrumental Analysis.

Optical methods of analysis.

Practical classes

Practice 1

Gravimetry.

Practice 2

Acid-base titration.

Practice 3

Rating Complexometric.

Practice 4

Redox titration.

Practice 5

Precipitation ratings.

Practice 6

Spectrophotometric determinations.

Practice 7

Practical Exam.

5273 INORGANIC CHEMISTRY (I)

Topic 1

Introduction to Inorganic chemistry.

Inorganic chemistry: concept, evolution, current situation. Relationship with other disciplines. Presentation as a subject: contents, organization and structure, objectives, development, methodology, evaluation. Introduction to descriptive Inorganic Chemistry. Trends in chemical properties of the elements and their compounds.

Topic 2

Hydrogen.

Distribution. Isotopes. Spin isomers: ortho and para for hydrogen. Ions. Atomic and physical properties. Preparation, industrial procurement and applications. Chemical behavior. Hydrides: ionic (saline), (polymeric), covalent (molecular) and interstitial (metallic). Hydrogen bridge bonds. Enlargement: applications, energy of the future.

Topic 3

Group 1: Alkali Metals.

General characteristics, abundance, extraction or localization, uses and properties. Liquid ammonia dissolutions. Hydrides. Halides. Oxygenated combinations: oxides, peroxide, superoxides, suboxides, hydroxides and oxyalts. Complex compounds: crown ethers, cryptates, organometallic.

Extension: applications, biological importance, the chloroalkali industrial process (including Solvay process).

Topic 4

Group 2: Alkaline Earth Metals

General characteristics, abundance, extraction or obtaining, uses and properties. Beryllium chemistry. Hydrides. Halides. Oxygenated combinations: oxides, hydroxides and oxysalts. Complex compounds: organometallic, Grignard reagents.

Extension: Applications, biological importance, cements.

Topic 5

Group 12: Zinc, cadmium and mercury.

General characteristics, abundance, extraction or obtaining, uses and properties. Formal oxidation states: combinations of M^{2+} + elements, divalent compounds. Complex compounds: organometallic. Extension: applications, biological importance, batteries, environment.

Topic 6

Group 13: boron, aluminum, gallium, indium, and thallium.

Historical introduction. Abundance and distribution. Physical and chemical properties of the elements. Preparation and applications. Properties of some relevant compounds (borides, hydrides, halides, oxides and oxycompounds, alums). Complexes. Organometallic compounds. Bio-Inorganic Chemistry.

Topic 7

Group 14: carbon, silicon, germanium, tin, and lead.

Historical introduction. Abundance and distribution. Carbon allotropes: diamond, graphite (and its collation compounds), fullerenes and derivatives. Physical properties and chemical elements. Carbides and silicides. Hydrides. Halides (fluorocarbons and freons) and oxyhalides. Oxides and hydroxides. Carbonates. Silicates, aluminosilicates, zeolites and molecular sieves. Chalcogenides, cyanides and derivatives.

Metal clusters. Complexes. Organometallic compounds: Organic derivatives and silicon. Bioinorganic and environmental chemistry (greenhouse effect and destruction of the ozone layer).

Topic 8

Group 15: nitrogen, phosphorus, arsenic, antimony, and bismuth.

Historical introduction. Abundance and distribution. Physical and chemical properties of the elements. Production and uses. Nitrides, phosphides,



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arsenides and derivatives. Azides. Hydrides, hydrazine, hydroxylamine and derivatives. Halides, Oxyhalides and derivatives. Oxides and Oxycompounds. Oxyacids and oxysalts. Sulfides. Phosphorus compounds and nitrogen. Complex. Dinitrogen as a ligand. Organic derivatives. Bioinorganic and environmental chemistry.

Topic 9

Group 16: Oxygen, sulfur, selenium, tellurium, polonium.

Historical introduction. Abundance and distribution. Allotropes. Physical properties and chemical elements. Production and uses. Hydrides: water, hydrogen peroxide and others. Halides. Oxyhalides. Oxides. Oxyacids, Oxysalts. Sulfides, Selenides and tellurides. Sulfur and nitrogen compounds. Organic derivatives. Bio-inorganic and environmental chemistry.

Topic 10

Group 17: Halogens.

Introduction, abundance and distribution. Physical and chemical properties of the elements. Load transfer complexes. Production and uses. Interhalogenated compounds, polyhalides and cationic derivatives. Chlorine, bromine and iodine oxides. Oxyacids and their salts. Bioinorganic and environmental chemistry.

Topic 11

Group 18: Noble gases.

Introduction, abundance and distribution. Physical and chemical properties of Elements. Production and uses. Xenon, krypton and argon compounds.

5274 PHYSICAL CHEMISTRY (I): QUANTUM MECHANIC.

Topic 1

Concept of physical chemistry.

Review of previous knowledge: Preliminary physics and mathematics.

Assumptions of quantum mechanics.

The Schrödinger equation, results and solution for simple systems and hydrogenide atoms.

Interpretation of the wave function.

Angular moments of hydrogenide atoms.

Topic 2

The Schrödinger equation and its solution for polyelectronic systems.



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Approximate methods of Quantum Mechanics: method of variations and method of time-independent disturbances.

Anti-symmetric function: Slater determinant.

Approximate orbital of Slater. Angular magnetic moments of polyelectronic atoms:

Links. Symbols of the electronic states of atoms.

Atomic emission spectra. Selection rules.

Topic 3

Quantum mechanical study of the molecules. Born-Oppenheimer approximation.

Diatomic molecules.

Molecular Orbital method (OM). Angular momentum couplings.

Symbols of the electronic states of diatomic molecules. Selection rules.

Valencia Liaison Method (EV).

Polarity of the link. Comparison of molecular orbital theories and the bond valence method (BVM).

Topic 4

Polyatomic molecules. Molecular geometry. Directed valence.

Hybridization.

Multiple-link molecules. Conjugation and aromaticity.

Hückel approximations (HM).

5275 PHYSICAL CHEMISTRY (II): SPECTROSCOPY AND STATISTICAL THERMODYNAMICS

Molecular symmetry

Topic 1: Molecular symmetry.

Symmetry elements and operations. Classification of molecules according to their symmetry. Symmetry groups, subgroups, and classes. Matrix nomenclature.

Representations of groups. Character table. Representation of 3N Cartesian displacement vectors. Cyclic group representations

Basics of spectroscopy

Topic 2: Basic Principles of spectroscopy.

Introduction. Selection rules. Spectroscopic transitions. Absorption photometry.

Reason signal-noise, resolution and width. Areas of the spectrum.

Topic 3: Microwave spectroscopy.

Introduction. Rigid Rotor. Intensity of the bands. Non-rigid rotor. Stark effect.

Classification of molecules.

Topic 4: Infrared and Raman spectroscopy.



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Infrared spectroscopy. Vibration: diatomic molecules. Anharmonicity. Polyatomic molecules. Population of vibration levels. Vibration and Rotation: diatomic molecules. Influence of vibration on rotation. Isotopic effect.

Linear polyatomic molecules. Effect of nuclear spin. Other molecules

Polyatomics. Raman spectroscopy: Raman pure rotation spectrum. Raman rotational-vibrational spectrum. Active vibrations in Raman. Symmetry of normal modes of vibration.

Topic 5: UV-Vis spectroscopy.

Absorption spectroscopy. Diatomic molecules: vibrational base structure. Progressions. Franck-Condon principle. Energy and dissociation products. Fine rotational structure. Polyatomic molecules: main types of electronic transits. Location and delocalization of electrons. Applications. Emission spectroscopy: Introduction. Photophysical and photochemical processes. Quantum yields. Kinetics of photophysical processes: processes of interconversion between states and bimolecular deactivation (Quenching). Equation of Stern-Volmer.

Topic 6: Spin resonance spectroscopy

Nuclear magnetic resonance: nuclear magnetic moments. Energies of nuclei in magnetic fields. Chemical displacement. Fine structure, coupling. Electronic spin resonance: the g factor. Hyperfine structure.

Statistical thermodynamics

Topic 7: Non-localized independent particles.

The ideal gas as an assembly of independent non-localized particles: equation of state. Contribution of partition functions to energy, specific heat and entropy. Principle of equipartition of energy. Ideal gas mixture: evaluation of equilibrium constants.

Topic 8: Real Gases.

Introduction. Classic partition function. Maxwell-Boltzmann law of speed distribution. Intermolecular forces. Integral configuration. Equation of state: Elementary considerations. Virial equation. Intermolecular potential: Rigid Spheres, Lennard-Jones, Stockmayer and Kihara. Second Virial coefficient in terms of the configuration Integral.

Topic 9: Localized independent particles.

The atomic crystal as an assembly of independent localized particles. Classic C_v theory: Rules of Dulong-Petit, Kopp-Newman and Debye. The vibrational partition function: Einstein model. Limitations. Debye model. Limitations. Entropy of crystalline solids. Residual entropy.

5276 INORGANIC CHEMISTRY LABORATORY

PRACTICE 1

Elements of Group 1

SYNTHESIS: Preparation of $\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$ and Na_2CO_3 from NaHCO_3 .

REACTIVITY: Check the color of the flame produced by salts of Li, Na and K.

Addition of concentrated HCl to a saturated NaCl dissolution in water. Addition



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of EtOH on the saturated solution of NaCl in water. Li_2CO_3 solubility in water and reaction with HCl; verify compound precipitation by adding HCl concentrate or EtOH. Addition of HClO_4 to solutions of NaCl and KCl.

PRACTICE 2

Elements of Group 2

SYNTHESIS: Preparation of $(\text{NH}_4)_2\text{MgPO}_4 \cdot 6\text{H}_2\text{O}$ and $\text{Mg}_2\text{P}_2\text{O}_7$.

REACTIVITY: Mg behavior in the presence of water. Relative solubility of the hydroxides of Mg, Ca and Ba and reactivity in front of a soluble sulfate. Compare the different behavior of dissolutions of MgCl_2 and BaCl_2 versus NaOH, NH_4OH , H_2SO_4 and K_2CrO_4 .

PRACTICE 3

Elements of Group 12

SYNTHESIS: Preparation of HgI_2 .

REACTIVITY: Treat zinc grit with a few drops of concentrated HCl and with a few drops of HNO_3 concentrated in two different test tubes. Treat Zn with a few drips of NaOH 4M. Place ZnSO_4 solutions, $\text{Cd}(\text{AcO})_2$ and HgCl_2 in different test tubes and add copper thread. Place ZnSO_4 , $\text{Cd}(\text{AcO})_2$ and HgCl_2 in different test tubes and add NaOH. Place ZnSO_4 , $\text{Cd}(\text{AcO})_2$ and HgCl_2 in different test tubes and add NH_4OH . Place ZnSO_4 , $\text{Cd}(\text{AcO})_2$ and HgCl_2 in different test tubes and add Na_2S ; add HCl or HNO_3 to the precipitates once obtained. Place ZnSO_4 , $\text{Cd}(\text{AcO})_2$ and HgCl_2 in different test tubes and add KI. Place in two test tubes $\text{Hg}_2(\text{NO}_3)_2$ and add $\text{Na}(\text{OH})$ and KI.

PRACTICE 4

Elements of group 13

SYNTHESIS: Preparation of $\text{B}(\text{OH})_3$.

REACTIVITY: Determine the PH of a solution of $\text{B}(\text{OH})_3$, add glycerin and re-measure. Flame coloration of a boric ester. Behavior of aluminum in the presence of H_2O , HCl, HNO_3 , NaOH and NH_4OH . Treat a solution of $\text{Al}_2(\text{SO}_4)_3$ with NaOH, Na_2CO_3 and Na_2S . Microscale aluminothermy.

PRACTICE 5

Elements of Group 14

SYNTHESIS: Preparation of $\text{Pb}(\text{NO}_3)_2$.

REACTIVITY: Test the reactivity of $\text{Pb}(\text{NO}_3)_2$ versus HCl, H_2SO_4 , NaOH, NH_4OH , Na_2CO_3 , Na_2S , K_2CrO_4 and KI. To test the reactivity of SnCl_2 against HCl, H_2SO_4 , NaOH, NH_4OH , Na_2CO_3 , Na_2S , K_2CrO_4 and KI. Behavior of the Pb and Sn versus acid HCl.

PRACTICE 6

Elements of Group 15

SYNTHESIS: Preparation of NH_3 and a study of its reactivity against sodium.



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REACTIVITY: Determine the pH of aqueous dissolutions of NH_4Cl and $(\text{NH}_4)\text{AcO}$. Add a few drops of NaOH to a concentrated dissolution of NH_4Cl . Heat the solid NH_4Cl in a tube. Mix the concentrated NaNO_2 and NH_4Cl solutions and gently warm. Treat NaNO_2 with KMnO_4 and a few drops of AcOH . Treat NaNO_2 with KI , add a few drops of AcOH and add CCl_4 . Determine the PH of a solution of Na_3PO_4 . Obtaining Regia Water.

5277 ORGANIC CHEMISTRY (II)

Structural Determination II

Proton Nuclear Magnetic resonance spectroscopy

Introduction. Chemical displacement, resonance signal integration. Spin Systems. Proton coupling attached to heteroatoms. Application of Proton NMR to the structural elucidation of organic compounds.

Carbon-13 Nuclear Magnetic resonance spectroscopy

Introduction. Analysis of ^{13}C NMR spectra. Chemical displacement of Carbon-13 families of organic compounds. Application of ^{13}C NMR spectra to the structural study of organic compounds.

Organic Reactions II

Reactions on carbonylic and referable compounds. Aldehydes, ketones, imines, nitriles, cetenes, isocyanates

Nucleophilic addition reactions on the carbonyl group. General aspects. Factors that affect nucleophilic addition reactions. Stereochemistry of the addition reactions. Enols and Enolates. Reactions of synthetic interest: Interconversion of functional groups and formation of new carbon-carbon bonds.

Conjugated nucleophilic addition reactions. General aspects. Factors that affect conjugated addition reactions. Reactions of synthetic interest.

Reactions between carboxylic compounds and derivatives.

Nucleophilic substitution reactions at unsaturated carbon. General aspects. Factors affecting nucleophilic substitution reactions at unsaturated carbon. Reactions of synthetic interest: interconversion of functional groups and formation of new carbon-carbon bonds.

Homolytic reactions.

General aspects. Factors affecting homolytic reactions. Reactions of synthetic interest.

Molecular transpositions.

General aspects. Reactions of synthetic interest.



5278 INSTRUMENTAL ANALYSIS

OPTICAL METHODS OF ANALYSIS. Chapter I: Introduction to optical methods of analysis.

Topic 1. Fundamentals of optical methods of analysis.

Introduction.

Ondulatory properties of electromagnetic radiation.

Mechanical-quantum properties of electromagnetic radiation.

Fundamentals of interaction electromagnetic radiation-matter.

Classification of optical methods of analysis.

Topic 2. Optical analysis instruments.

Introduction.

General outline of optical analysis equipment.

Radiation sources.

Wavelength selectors.

Sample cells.

Radiation detectors.

Signal processor and reading devices.

Spectroscopic instrument designs.

OPTICAL METHODS OF ANALYSIS. Chapter II: Spectroscopic Methods

Topic 3. Methods based on the absorption of UV-visible radiation.

Introduction.

Analytical fundamentals of the UV-Visible radiation absorption process.

Comparison of the methods of atomic absorption and methods of molecular absorption.

Instrumentation.

Analytical applications.

Topic 4. Methods based on the emission of radiation in the UV-visible.

Introduction.

Analytical fundamentals of emission methods and photoluminescent methods.

Comparison of atomic emission and molecule emission methods.

Instrumentation.

Analytical applications.

Topic 5. Methods based on infrared radiation absorption.

Introduction.

Analytical fundamentals of the infrared absorption process.

Instrumentation

Analytical applications.

Topic 6. Methods based on radiation dispersion.

Introduction.



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Analytical fundamentals of the phenomenon of radiation dispersion.
Turbidimetry and Nephelometry
Raman spectroscopy.
Analytical applications.

ELECTROANALYSIS. Chapter IV: Introduction to electrochemical methods of analysis.

Topic 7. Introduction to Electrochemistry.

Introduction.

Concept of electroanalysis.

The electrochemical cell.

Faradaic processes.

The nature of the electrode-solution interface. Non-Faradaic processes.

Potential for liquid bonding.

Variables that affect an electrochemical experiment

Classification of electroanalytical techniques.

Instrumentation.

Topic 8. General characteristics and stages of the electrode reaction.

Introduction.

Stages of the electrode reaction.

Electronic transfer.

Mass transport.

Chemical reactions prior to and after the exchange of electrons.

Surface processes on the electrode.

ELECTROANALYSIS. Chapter V: Electroanalytic techniques.

Topic 9. Steady-state techniques and total electrolysis techniques.

Introduction.

Amperometric evaluation.

Coulometry.

Electrogravimetry.

Potentiometry.

Conductimetry.

Applications.

Item 10. Techniques in a non-stationary state.

Introduction.

Chronoamperometry.

Chronocoulometry.

Voltamperometry.

Pulse Techniques

Chronopotentiometry.

Applications.

Topic 11. Resolution techniques.

Introduction.

General resolution techniques.

Voltammetric stripping analysis.

Potentiometric stripping analysis.

Quantification.

Interference.

Analytical applications of stripping analysis.

Practices

Laboratory practices

During the practical sessions, the student will use the standard instrumental techniques in the analytical chemistry laboratory (absorption spectrophotometry Molecular and atomic, flame photometry, Potentiometry, voltammetry, etc...).

5279 INORGANIC CHEMISTRY (II).

Unit 1

1. Introduction to the chemistry of coordination.

Historical development. Coordination numbers and geometry. Polymetallic complexes. Classification of ligands by type of link that generate, σ , π , donors, acceptors and non-innocents, and by the coordination positions that they occupy. Neutral and charged ligands, monodentate, polydentate, bridges and chelators. Isomers: bonding, ionization, hydrating, coordination and stereoisomerism. Oxidation states, electronic configurations and "d" electron counts. Comparison of the elements of the first transition series (d-block) by their electronic configuration dn .

2. Group theory and bonding models in coordination compounds.

Crystalline field theory. Magnetic and electronic properties. Use of the table of characters. Molecular orbital theory. Ligands π donors and/or acceptors. Model of angular overlap. Energy factors that determine the number and the coordination geometry.

3. Stability of coordination compounds.

Staggered and total formation constants. Factors that affect stability. Nature of the metallic ion: classes a, b and limit. Nature of the ligand. Irving-Williams series. Chelate and macrocyclic effects. Influence of stability constants in redox chemistry.

4. Mechanisms of the reactions of the coordinating compounds (I).

Transfer reactions of atoms and groups of atoms. Mechanisms D, A, I. The determining speed stage: Da , Dd , Aa , Ad , Ia , Id . Criteria for assigning mechanisms. Factors affecting the reactivity of plane squared complexes:

Nature of the incoming ligand (nucleophile), trans effect, cis effect, nature of the central ion. Substitution reactions in octahedral complexes. The Eigen Wilkins mechanism.

Stereochemistry of substitution. Hydrolysis catalyzed by bases: mechanism of the conjugate base. Template synthesis.

5. Mechanisms of the reaction of the coordinating compounds (II).

Electronic transfer reactions. External sphere mechanisms (tunnel process). Autoexchange reactions. The equation of Marcus and Marcus-Hush. The Marcus inverted region. Internal sphere mechanisms. Transfer of two electrons. Applications of electronic transfer reactions. Electronic transfer in excited states. Redox photochemical reactions. Damping of excited states. Chemiluminescent. Design of a photoelectrochemical cell. Intramolecular Electronic transfer: Mixed valence bonds.

Unit 2

6. Bioinorganic.

Applications of complex formation reactions complex and electronic transference in biological processes. Objectives of bio-inorganic chemistry. Functions of inorganic species in biological systems. Macroelements and trace elements: essentiality and toxicity. Bioavailability. Recruitment and transformation of inorganic elements into living organisms. Oxygen transport and storage: haemoglobin and myoglobin. Nitrogen fixation: Molybdenum nitrogenase. Vitamin B12. Sensors. Medical applications.

7. Organometallic compounds.

Historical development. Rule of 18 and 16 electrons. Ligands and electrons counts: covalent system and neutral ligand and ionic system or pair donor. Metal carbonyls. Group frequencies and infrared characterization of carbonyls. "Clusters" and rules of Wade-Mingos-Lahuer (PSEPT-TPEEP: Polyhedral skeleton electron pair theory). Compound types according to the ligand: alkyls and aryls, alkenes and alkynes and non-conjugated dienes. Allyls and Cyclopentadienyl radicals. Alkanes, Agostic hydrogens and noble gases. Reactions of the organometallic compounds of transitional metals.

8. Solid-State chemistry (I).

Crystalline state and defects. Description of the ideal crystals. Representations by networks of polyhedra. Point defects, linear defects and extensive defects. Non-stoichiometric solids. Thermodynamic and structural aspects. Composition intervals in non-stoichiometric phases. Assimilation and elimination of defects. Solid solutions.

9. Solid-State chemistry (II).

Preparation methods. General principles. Experimental procedures. Preparation of precursors for solid-state reactions: coprecipitation. Kinetics of solid-state reactions. Crystallization of solutions, melted, glasses and gels. Methods of transport in gaseous phase: "Chemical vapor deposition". Modifications of existing structures through ion exchange reactions and intercalation. Methods of electrochemical reduction. Preparation of thin layers. Growth of Monocrystals. Methods of high pressures and hydrothermal synthesis.

10. Homogeneous and heterogeneous catalysis.

Nature of the catalysts. Catalytic cycles and stages. Hydrogenation and Hydroformulation of alkenes. Ammonia synthesis. Oxidation of SO₂. Interconversion of aromatic compounds by zeolites. Electrocatalysis.

11. Nanomaterials, nanoscience and nanotechnology.

Manufacturing and characterization. Materials arranged in layers. Self assembly and supramolecular chemistry. Organic-inorganic hybrid nanocomposites. Bio-organic nanomaterials.

12. Laboratory practices.

5280 PHYSICAL CHEMISTRY III: CHEMICAL THERMODYNAMICS

1. Thermodynamics in multicomponent systems.

Introduction. Units of concentration. Condition of additivity, study in a mixture of ideal gases, molar properties. Partial molar properties. Average molar property. Apparent molar property. Other properties of the partial molar properties. Methods for their determination.

2. Chemical potential.

Definition and characteristics. Chemical potential as an equilibrium criterion. Explicit form of chemical potential. Application to ideal gas mixtures. General expression of the chemical potential and deduction of its value for the standard state.

3. Ideal solutions.

Ideal solutions. Raoult's law. The thermodynamic magnitude of the mixing process. Liquid-vapor equilibrium in ideal solutions. Ideal solubility of gases and solids. Ideal diluted solution. Henry's law. Binding properties. Distribution of a solute between two immiscible solvents.

4. Non-ideal solutions for non-electrolyte.

Non-ideal solution types. Potential non-ideal chemical solutions. Thermodynamic functions of excess. Determination of activities and coefficients of activity. Gibbs-Duhem equation. Duhem-Margules equation. Coefficients of activity at different concentration scales.

5. Phase changes in pure substance systems.



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Multi-phase systems of a component. Phase stability. Phase transitions. First Order: Clapeyron and Clausius-Clapeyron equations. Diagrams of phases of pure substances. Effect of pressure on vapor pressure. Transitions. Higher-order phases.

6. Binary liquid systems. Phase changes in multicomponent systems.

Homogeneous systems in liquid phase. Application of the phase rule. Liquids. Totally immiscible. Diagrams pressure-composition and temperature-composition. Liquid vapor equilibrium. Lever rule. Immiscible Binary Systems and partially miscible. Distillation.

7. Electrolyte Solutions.

Electrolyte solutions as non-ideal systems. Chemical potentials of electrolytes. Average ionic magnitudes. Experimental determination of the electrolyte activity coefficients. Divergence of the coefficients of activity with respect to the boundary laws of the binding properties.

8. Thermodynamics of electrochemical cells.

Introduction. The electrified interface. Electrochemical potential. Materialization of an electrochemical battery, Nernst equation. Factors that influence the potentials. Battery applications.

9. Surface thermodynamics and adsorption.

Surface phenomena. Surface and interfacial tension. Vapor pressure in curved surfaces: Young-Laplace equation and Kelvin equation. Capillarity. Experimental measurement of surface tension. Gibbs Interfaces Model: Gibbs adsorption isotherm. Surface adsorption: isotherms of Langmuir, Freundlich, and Temkin.

Laboratory experimentation

Perform three lab practices between:

- Volumetric properties.
- Phase equilibrium.
- Chemical equilibrium.
- Surface phenomena.

5281 NUMERICAL ANALYSIS AND APPLIED STATISTICS

Block 1. Regression and design of experiments

Introduction to the theory and the applications of statistics

- Univariate regression. Application to calibration and comparison methods.
- Linear and nonlinear multivariate regression.

Introduction to design of experiments

- Screening and factorial experiments.
- Response surface methods.

-Experimental optimization.

Block 2. Computational methods

Numerical optimization methods

Iterative methods in one and several variables.

Experimental data processing by computer

-Signal processing. Signal/noise ratio. Savitzky-Golay filters.

-Application of the derivative to improve the quality of the signal.

Simulation

Monte Carlo Method: Simulation. Markov Chain-based sampler (MCMC).

➤ **3rd year**

5282 ORGANIC CHEMISTRY III: ORGANIC SYNTHESIS

1. INTRODUCCIÓN TO ANALYTICAL SEPARATION TECHNIQUES

TOPIC 1.-GENERAL INFORMATION ON SEPARATION TECHNIQUES

- * Separation techniques in the analytical process.
- * Classification of analytical separation techniques.
- * Fundamentals of separation processes.
- * Parameters of interest in analytical separation techniques.
- * Errors associated with separation processes.

NON-CHROMATOGRAPHIC SEPARATION TECHNIQUES

TOPIC 2.- SEPARATION BY EXTRACTION

- * Introduction to extraction separation methods.
- * Liquid-liquid extraction.
 - Liquid-liquid extraction techniques.
 - Applications.
- * Solid-liquid extraction.
 - Soxhlet extraction.
 - Ultrasonic assisted extraction.
 - Microwave extraction.
- * Extraction with supercritical fluids.
 - Definition and properties of supercritical fluids.
 - Choice of supercritical fluid.
 - Instrumentation in supercritical fluids.
 - Applications.



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- * Solid phase extraction and microextraction.
- Stages and foundation of solid phase extraction.
- Solid phase microextraction.

TOPIC 3.- IONIC EXCHANGE

- * Introduction and fundamentals of ion exchange.
 - * Classification of Ion exchangers. Ion exchange resins.
- Properties.
- * Ion exchange equilibrium.
 - * Kinetics of ion exchange.
- Applications.

CHROMATOGRAPHIC SEPARATION TECHNIQUES

TOPIC 4.-INTRODUCTION TO CHROMATOGRAPHIC SEPARATION TECHNIQUES

- * General description of chromatography.
 - * Classification of chromatographic separation techniques.
- Chromatograms.
- * Retention time. Distribution coefficient. Retention Factor.
 - * Column efficiency and band widening. Kinetic theory of chromatography.
 - * Separation of mixtures. Separation Factor. Definition and optimization of the Resolution.
 - * Chromatographic applications.

TOPIC 5.-GAS CHROMATOGRAPHY

- * Fundamentals of gas chromatography.
 - * Instrumentation in gas chromatography. Carrier Gas: Types and properties.
- Sample Introduction System. Columns and stationary phases. Control of Temperature. Detectors.
- Derivatization.
- * Purge and trap. Headspace.
- Applications.

TOPIC 6.-LIQUID CHROMATOGRAPHY

- * Column Chromatography.
 - * High-resolution liquid chromatography (HPLC).
- Instrumentation in HPLC. Mobile phase supply and storage system.
- Mobile phase Drive system. Sample injection systems.
- Columns in HPLC.
- Detectors in HPLC.
- Fundamentals and applications of the different types of Column Chromatography.
- Partition chromatography. Adsorption chromatography. Chromatography of Ion Exchange. Exclusion chromatography by size. Affinity Chromatography.
- * Flat chromatography.
- Theory of flat chromatography and applications.



TOPIC 7.-Supercritical fluid chromatography

- * Introduction to supercritical fluid chromatography.
- * Mobile phase and stationary phase.
- * Instrumentation in supercritical fluid chromatography.

Applications.

- * Comparison with other chromatographic methods.

ELECTROPHORETIC SEPARATION TECHNIQUES

TOPIC 8.-ANALYTICAL TECHNIQUES OF ELECTROPHORETIC SEPARATION

- * Theory of electrophoretic separations. Electromigration and Electroosmosis. Types of techniques.
- * Capillary electrophoresis. Foundation. Instrumentation. Efficiency and resolution.
- * Types of capillary electrophoresis. Zonal capillary electrophoresis. Capillary gel electrophoresis.
- * Capillary Isoelectric focusing. Capillary Isotachophoresis.

**5283 SEPARATION TECHNIQUES in ANALYTICAL
CHEMISTRY.**

INTRODUCTION TO ANALYTICAL SEPARATION TECHNIQUES

TOPIC 1.-GENERAL INFORMATION ON SEPARATION TECHNIQUES

- * Separation techniques in the analytical process.
- * Classification of analytical separation techniques.
- * Fundamentals of separation processes.
- * Parameters of interest in analytical separation techniques.
- * Errors associated with separation processes.

NON-CHROMATOGRAPHIC SEPARATION TECHNIQUES

TOPIC 2.- SEPARATION BY EXTRACTION

- * Introduction to extraction separation methods.
- * Liquid-liquid extraction.
 - Liquid-liquid extraction techniques.
- Applications.
- * Solid-liquid extraction.
 - Soxhlet extraction.
 - Ultrasonic assisted extraction.
 - Microwave extraction.
- * Extraction with supercritical fluids.
 - Definition and properties of supercritical fluids.



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- Choice of supercritical fluid.
- Instrumentation in supercritical fluids.
- Applications
 - * Solid phase extraction and microextraction.
- Stages and foundation of solid phase extraction.
- Solid phase microextraction.

TOPIC 3.-ION EXCHANGE

- * Introduction and Fundamentals of ion exchange.
 - * Classification of Ion exchangers. Ion exchange resins. Properties.
 - * Ion exchange equilibrium.
 - * Kinetics of ion exchange.
- Applications.

CHROMATOGRAPHIC SEPARATION TECHNIQUES

TOPIC 4.-INTRODUCTION TO CHROMATOGRAPHIC SEPARATION TECHNIQUES

- * General description of chromatography.
- * Classification of chromatographic separation techniques.
- * Chromatograms.
- * Retention time. Distribution coefficient. Retention Factor.
- * Column efficiency and band widening. Kinetic theory of chromatography.
- * Separation of mixtures. Separation factor. Definition and optimization of resolution.
- * Chromatographic applications.

TOPIC 5.- GAS CHROMATOGRAPHY

- * Fundamentals of gas chromatography.
 - * Instrumentation in gas chromatography. Carrier Gas: Types and properties.
- Sample Introduction System. Columns and stationary phases. Temperature control. Detectors. Derivatization.
- * Purge and trap. Headspace.
- Applications.

TOPIC 6.-LIQUID CHROMATOGRAPHY

- * Column chromatography.
 - * High-resolution liquid chromatography (HPLC).
- Instrumentation in HPLC. Mobile phase supply and storage system.
- Mobile phase drive system. Sample injection systems.
- Columns in HPLC.
- Detectors in HPLC.
- Fundamentals and applications of the different types of column chromatography.
- Partition chromatography. Adsorption chromatography. Ion exchange chromatography. Exclusion chromatography by size. Affinity chromatography.
- * Flat chromatography.
- Theory of flat chromatography and applications.



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TOPIC 7.- SUPERCRITICAL FLUID CHROMATOGRAPHY

- * Introduction to supercritical fluid chromatography.
 - * Mobile phase and stationary phase.
 - * Instrumentation in supercritical fluid chromatography.
- Applications.
- * Comparison with other chromatographic methods.

ELECTROPHORETIC SEPARATION TECHNIQUES

TOPIC 8.- Analytical techniques of electrophoretic separation.

- * Theory of Electrophoretic separations. Electromigration and Electroosmosis. Types of techniques.
- * Capillary electrophoresis. Foundation. Instrumentation. Efficiency and resolution.
- * Types of capillary electrophoresis. Zonal capillary electrophoresis. Capillary gel electrophoresis.
- * Capillary Isoelectric focusing. Capillary Isotachophoresis.

5284 PHYSICAL CHEMISTRY LABORATORY

I-THERMODYNAMIC BLOCK:

Mix properties.
Binding properties.
Activity coefficients.
Liquid-liquid equilibrium.
Saline effect.
Electrochemistry.
Conductimetry.
Potentiometry.
Spectroscopy.
Calorimetry.

II-KINETIC BLOCK:

Determination of the reaction order and the speed constant.
Effect of temperature.
Catalytic effect.

III-GENERIC BLOCK

Atomic spectra.
Spectroscopy.

5285 PHYSICAL CHEMISTRY IV: CHEMICAL KINETICS

Fundamentals of Chemical Kinetics

TOPIC 1: Reaction speed.

Rational and experimental definitions.-Velocity equation.-Molecularity.-
Simple reactions.-Reaction order.-Influence of temperature on the reaction rate.-
Experimental methods.

TOPIC 2: STUDY OF COMPLEX KINETIC PROCESSES.

Reversible reactions, simultaneous, consecutive, chain reactions.- Stationary Regime
method.-Determining stage.

TOPIC 3: Collision method.

Introduction. -Characteristics of the molecular shocks. -Number of effective collisions. -
Bimolecular reactions.

TOPIC 4: Transition state method.

Introduction. - Surfaces of potential energy. -Characteristics of the activated complex. -
General formulation of the theory. -Isotopic kinetic effects.

TOPIC 5: Reactions in solutions.

Influence of the solvent. -Brønsted-Bjerrum equation. - Reactions with the
participation of ions. Primary saline kinetic effect.

Catalysis

TOPIC 6: Homogeneous catalysis.

Characteristics of catalytic activity. - General mechanism of catalysis. -Types of
homogeneous catalysis in solution. -Acid-base catalysis. - Secondary saline kinetic
effect.

TOPIC 7: Heterogeneous catalysis.

Features. - Isotherm of Langmuir. Effective area of an adsorbent. - Stages of a
heterogeneous catalysis process. - Formal kinetics. - Heterogeneous catalysis
mechanism. - Activators and poisons.

5286 CHEMICAL ENGINEERING (I)

TOPIC 1. Introduction.

- 1.1. The chemical Industry: origins and evolution of chemical engineering.
- 1.2. Current and future trends in chemical engineering.
- 1.3. The chemical processes at present and prospects for the future.
- 1.4. Description, by way of example, of an industrial chemical process.
- 1.5. Systems of magnitudes and units. A dimensional number.



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TOPIC 2. Basic Operations of Chemical Processes.

- 2.1. Concept of basic operation.
- 2.2. Classification of basic operations.
- 2.3. Introduction to transport phenomena: molecular transport and turbulent transport.
- 2.4. Systems of magnitudes and units.

TOPIC 3. Material Balances.

- 3.1. General conservation equation of any extensive property.
- 3.2. Macroscopic balances of matter: general expression.
- 3.3. Macroscopic balances of matter in a stationary regime.
- 3.4. Macroscopic balances of matter in a non-stationary regime.

TOPIC 4. Energy balances.

- 4.1. Forms of energy expression.
- 4.2. Macroscopic energy balances: general expression.
- 4.3. Enthalpy balances.
- 4.4. Macroscopic energy balances in stationary and non-stationary regimes.

TOPIC 5. Fluid flows. Fluid flow-based operations.

- 5.1. Viscosity of fluids. Classification of fluids.
- 5.2. Basic equations in the internal flow of fluids. Energy losses by friction.
- 5.2. Power required for flow.
- 5.3. Measurement of flows.
- 5.4. Flow on porous beds.
- 5.5. Operations based on the external flow of fluids.

TOPIC 6. Heat transmission. Heat-transmission based operations.

- 6.1. Heat transmission mechanisms.
- 6.2. Heat conduction in simple geometry solids.
- 6.3. Convection heat transmission. Heat transmission coefficient.
- 6.4. Heat exchangers.
- 6.5. Evaporation. Evaporation by crystallization.

5287 BIOCHEMISTRY

UNIT I. INTRODUCTION TO BIOCHEMISTRY

TOPIC 1. Introduction

1. Concept and objectives of biochemistry. 2. Brief history of biochemistry.

UNIT II. CONFORMATION AND FUNCTION OF PROTEINS



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TOPIC 2.- Introduction to proteins. Structure and conformation of protein molecules

1. Functions and biological importance of proteins. 2. Structure and conformation of proteins. 3. Stabilizing links of the different levels of structure. Denaturing and folding. 4. Biocomputing-Databases.

TOPIC 3.- Structure and function of proteins

1. Concept and function of fibrous proteins. 1.1. Structure in helix- α . Keratins 1.2. Structure in β -pleated sheets. b. Silk fibroin. 1.3. Structure of collagen. 2. Reversible binding of a protein to a ligand: oxygen binding proteins. 2.1. Function and tertiary structure of myoglobin. 2.2. Function and quaternary structure of the Hemoglobin. 2.3. Differences between myoglobin and hemoglobin. 3. Complementary interactions between proteins and ligands: the immune system and immunoglobulins. 4. Protein interactions modulated by chemical energy: actin, myosin and molecular motors.

TOPIC 4.- Experimental methods for the study of proteins

1. Separation of proteins by size, solubility, load, and affinity. 2. Separation of proteins by electrophoresis. 3. Ultracentrifugation. 4. Determination of the primary protein structure. 5. Determination of the protein structure by X-ray crystallography. 6. Location and determination of proteins with antibodies.

TOPIC 5.- Enzymes: basic concepts and kinetics

1. Function and general characteristics of the enzymes. 2. Mode of action of the enzymes. 3. Kinetics of enzymatic reactions. Michaelis-Menten equation. Meaning of K_m and V_{max} . Spare number. Effect of pH and temperature. Reversible inhibition (competitive and non-competitive). Irreversible inhibition. Allosteric enzymes.

UNIT III. TRANSMISSION OF GENETIC INFORMATION

TOPIC 6.- Structure and DNA replication

1. Structure and characteristics of DNA. 2. Experimental methods for the study of nucleic acids. 3. Semi-conservative replication of DNA in prokaryotes. 4. Replication in eukaryotes.

TOPIC 7.- Biosynthesis and RNA maturation.

1. Structure and characteristics of the different types of RNA. 2. DNA transcription in *E. coli*. 3. Transcription in eukaryotes. 4. Maturation of the RNA.

TOPIC 8.- Translation: The genetic code and protein biosynthesis.

1. The genetic code. 2. Transfer RNA as an adapter molecule. 3. Structure, characteristics and role of ribosomes. 4. Global vision of the translation process. Stages 5. Protein biosynthesis. Differences in eukaryotes. 6 Post-translational maturation.

UNIT IV. BIOENERGETICS. GENERATION AND TRANSFORMATION AND USE OF METABOLIC ENERGY

TOPIC 9.-Introduction to metabolism. Principles of Bioenergetics.

1. Introduction to metabolism. 2. Types of metabolic pathways. 3. ATP role as an energetic intermediary. 4. Differences between NADH and NADPH. 5. Catabolism and Anabolism. 6. Central routes of energy metabolism.



TOPIC 10.-Regulation of metabolic pathways.

1. Control of the catalytic activity of enzymes 2. Control of the enzymatic concentration. 3. Regulation for substrate accessibility. Compartmentation. 4. Hormonal regulation of energy metabolism in mammals.

TOPIC 11.-Glycolysis, gluconeogenesis and pentose phosphate pathway.

1. Global vision of glycolysis. Location and energy efficiency. Anaerobic and aerobic glycolysis. Relationship with other pathways. 1.1. Phases and reactions of glycolysis. 1.2. Anaerobic glycolysis. 1.3. Regulation of glycolysis. 2. Gluconeogenesis. Global overview. 2.1. Pathway precursors. Reactions. 3. Coordinated regulation of glycolysis and the gluconeogenesis. Futile cycles. 4. Pentoses phosphate pathway. Global overview. Pathway function and location. 4.1. Reactions and relation with other metabolic pathways. 4.2. Control of the pentoses phosphate pathway.

TOPIC 12.-Glycogen metabolism

1. Glycogen as storage polysaccharide and glucose source. 2. Glycogen degradation. Entrance into the glycolysis. 3. Glycogen synthesis. 4. Coordinated regulation of phosphorylated glycogen and glycogen synthase.

TOPIC 13.-Citric acid cycle

1. Oxidative decarboxylation of pyruvate. pyruvate dehydrogenase complex. 2. Global vision of the citric acid cycle. 3. Cycle reactions. 4. The cycle as a source of biosynthetic precursors. The glyoxylate cycle. 5. Regulation of the pyruvate dehydrogenase complex and the citric acid cycle.

TOPIC 14.-Oxidative phosphorylation and photophosphorylation

1. Global overview. Cellular localization. 2. Oxidative phosphorylation. 2.1. Enzymatic electron transport chain complexes. 2.2. Protomotor force and ATP synthesis. 2.3. Uncoupling agents. 2.4. Glycerol-3-phosphate and malate-aspartate shuttles. 2.5. Regulation of oxidative phosphorylation. 2.6. Energy efficiency of oxidative phosphorylation. 3. General characteristics of photophosphorylation. 3.1. Light-driven electronic flux. 3.2. ATP synthesis by photophosphorylation.

TOPIC 15.-Biosynthesis of carbohydrates in plants

1. Photosynthetic reduction cycle of carbohydrates. Calvin cycle. 1.2. CO² fixation and sugar production. 1.3. Regeneration of the acceptor molecule ribulose.

TOPIC 16.-Metabolism of fatty acids and lipids

1. Global Vision. 2. Oxidation of fatty acids. 3. Biosynthesis of fatty acids.

TOPIC 17.-Amino acid metabolism and urea cycle

1. Degradation of dietary proteins to amino acids. 2. Deamination of amino acids. 3. Nitrogen excretion. 4. Degradation of carbon skeletons of the amino acids.

5288 ORGANIC CHEMISTRY LABORATORY

Introductory seminars to organic synthesis

Application of spectroscopic analysis techniques for structural determination of compounds that will be synthesized. NMR spectroscopy. Gases/Mass chromatography. Experimental techniques in organic synthesis

Transformation of functional groups

- Practice 1: Oxidation reactions.
- Practice 2: Reduction reactions.
- Practice 3: Introduction to Green Chemistry.

Carbon-carbon link formation

- Practice 1: Addition and condensation aldolization reactions.
- Practice 2: Diels-Alder cycloaddition reactions.
- Practice 3: Organometallic compounds: Preparation of magnesians and addition reactions to carbonylic compounds.
- Practice 4: Direct nucleophilic substitution reactions of alcohols.
- Practice 5: CC double-bond forming reactions.
- Practice 6: Transition metal-catalyzed reactions.

Formation of carbon-hetero links

- Practice 1: Electrophilic aromatic substitution.
- Practice 2: Cycloaddition 1.3-dipolar reactions.
- Practice 3: Multicomponent reactions.
- Practice 4: Nucleophilic substitution: Synthesis of ethers and thioethers.
- Practice 5: Radicalary Addition: Synthesis of Alkenylsulfones.
- Practice 6: Nucleophilic substitution on unsaturated carbon: synthesis of carbamates

Synthesis of Heterocycles

- Practice 1: Synthesis of oxygenated heterocycles.
- Practice 2: Synthesis of nitrogenous heterocycles.
- Practice 3: Synthesis of sulfur heterocycles.

5289 CHEMOMETRICS AND EXPERIMENTATION IN ANALYTICAL CHEMISTRY

Theoretical program of the Subject

TOPIC 1. Validation of chemical measures.

Chemometrics and information in analytical chemistry.
Validation of an analytical procedure.
Quality parameters in regulated contexts: accuracy, veracity, precision, repeatability, reproducibility, sensitivity, linear range, detection limit, reliability and robustness.
A common analysis of some usual definitions (ISO, IUPAC).

TOPIC 2. Comparison of two analytical procedures.

Model for random and systematic errors.
Reference materials to assess bias.
Comparison of the veracity and accuracy of two procedures and/or methods of



analysis based on hypothesis testing.

Calculation of sample sizes to obtain the desired precision and veracity.

TOPIC 3. Multiple comparisons.

Determination of repeatability and reproducibility according to ISO-5725 by means of variance analysis.

Sources of variability of an analytical result.

Calculation of sample sizes in interlaboratory tests using Anova.

Purpose of the aptitude tests and the interlaboratory tests. Zscores analysis.

Detection of anomalous data in interlaboratory trials.

Test to compare multiple means. Variance homogeneity.

ANOVA of two or more factors: study of different effects and their interactions.

Approximation for factor interaction calculation.

Nested ANOVA: Assignment of variances to the different stages of a procedure and/or chemical process.

TOPIC 4. Linear calibration.

Applications of calibration models based on least squares regressions.

Distribution of calibration patterns in linear calibrations to optimize determination accuracy.

Analytical sensitivity.

Standard addition method.

Comparison of methods by linear regression.

Detection of anomalous data by robust regression: effect of anomalous data on the detection limit.

TOPIC 5. Ability to detect a method of analysis.

Definitions of the detection limit (ISO 11843, IUPAC, Decision 2002/657/CE).

Detection limit estimation methods based on a calibration.

Evaluation of the odds of false positive and false negative.

Decision limit.

Detection capability.

Operating curves.

TOPIC 6. Uncertainty calculations in an analytical procedure.

Uncertainty. Compound uncertainty.

Error propagation in uncertainty calculation.

Transmission of error: i) in linear functions; Non-linear functions of one or more variables; III) in the absence of a functional relationship.

Some analytical applications in complex procedures for calculating uncertainties.

TOPIC 7. Reliability and robustness of analytical procedures.

A priori control of the procedure: Plackett-Burman designs to evaluate robustness.

"A posteriori" control of the procedure: Control charts. Multivariate control charts.

TOPIC 8. Introduction to multivariate analysis.

Different levels of pattern recognition.

Main component concept and its usefulness in analytical chemistry.

Analysis in main components. Component interpretability.

Regression-based multivariate calibration on principal components.

Practical program of the subject

Laboratory practices

1. Optimization, through experimental design methodology, of liquid-liquid extraction. Extraction of iron with methyl-isobutyl-ketone.
2. Calculation of the recovery and determination of iron in mussels by flame atomic absorption spectrophotometry.
3. Determination of the decision limit and the detection capacity of an analysis procedure by UV/Visible molecular absorption spectrophotometry.
4. Evaluation of decision limit and detection capacity with selective electrodes. Chloride-selective electrode.
5. Control over time of various parameters (PH, chloride concentration and electrical conductivity) in the water supply network. Use of an automatic sampler.
6. Comparison of bleaching power of various powder-cleaning products.
7. Study of the effect of the sampling, dilution and measurement stages in the determination of an analyte. Evaluation of variability attributable to each stage. Calculation of individual and compound uncertainty according to ISO 5725.
8. Comparison of two analytical methods for copper determination.
- 9a. Analysis of the effect of several factors in the determination of propyl and methyl paraben by HPLC using a Plackett-Burman design.
- 9b. Analysis of robustness in the determination of ethanol and butanol in aqueous mediums by gas chromatography (CG) using a Plackett-Burman design for three experimental factors.
10. "Interlaboratory" (intergroup) analysis with the data obtained in their practices. Determination of repeatability and intermediate reproducibility. Detection of anomalous data by levels. Study of inter-group measurement homogeneity.
11. Study of the effect of two factors (analyst and sample) as well as their interaction on the results obtained when calculating the whitening power of a cleaning product in powder form by different students.
12. Group work: establishment of a working group for the implementation, analysis and discussion of the results obtained in Activity 5 by the different groups.
13. Principal Component Analysis (PCA) of samples of whisky to detect consumer product fraud.
14. Determination of copper by standard addition.

5290 INORGANIC CHEMISTRY (III)

Single Thematic Unit

TOPIC 1. Introduction

Introduction to the chemistry of transition elements. Transition elements in the periodic table: elements of Block d, elements of Group 12 and elements of Block f. Definition and characteristics of the elements of Blocks d and f. Specific trends of the transition elements.

TOPIC 2. Group 4: Ti, Zr and Hf.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, trends and chemical reactivity, and applications. Oxides. Piezoelectric effect of BaTiO₃. Sulfides. Halides. Complex. Ziegler-Natta catalysts in the polymerization of olefins. Sharpless catalysts in the enantioselective epoxidation of olefins.

TOPIC 3. Group 5: V, Nb and Ta.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, tendencies and chemical reactivity, and applications. Oxides. Sulfides. Oxyanion and Polyoxometalates (POM). Halides. Complex. Essentiality of V in some living organisms.

TOPIC 4. Group 6: Cr, Mo and W.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, trends and chemical reactivity, and applications. Oxides. Isopoly- and Hetero-polyanions (POM). Mo and W bronzes. Sulfides. Chevrel phases. Halides. Complexes. Multiple metal-metal bonds: Cr (II) acetate and quintuple M-M bond. Biological aspects of Cr and Mo.

TOPIC 5. Group 7: Mn, Tc and Re.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Oxyanions. Halides. Complexes. Role of Mn in photosynthesis (photosystem II). Use of ^{99m}Tc in Radiodiagnosis.

TOPIC 6. Group 8: Fe, Ru and Os.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Oxyanions. Halides. Complex. Prussian Blue. Biological aspects of iron.

TOPIC 7. Group 9: Co, Rh and Ir.

General aspects of the elements: Historical introduction, Abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Sulfides. Halides. Complexes. The Knowles and Noyori catalysts in enantioselective hydrogenation processes: synthesis of L-DOPA and naproxen.

TOPIC 8. Group 10: Ni, Pd and Pt.

General aspects of the elements: historical introduction, Abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Sulfides. Halides. Complexes. Cyclic polymerization of Reppe. Wacker process. Monsanto and Cativa processes. PdCl₂-based CO-Detectors. Cytotoxicity of Pt compounds.

TOPIC 9. Group 11: Cu, Ag and Au.

General aspects of the elements: historical introduction, Abundance and Distribution, ores and minerals, procurement, steelmaking and steels, physical properties, Trends and chemical reactivity, and applications. Oxides. Sulfides. Halides. Complex. Ag halides in photography. Blue copper proteins in Redox-type biological processes.

TOPIC 10. Group 3: Sc, Y, La and Ac, Lanthanides and actinide.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, tendencies and chemical reactivity, and applications. Most important compounds.

5291 STRUCTURAL METHODS IN INORGANIC CHEMISTRY

Block 1. Introduction

Block activities:

Initial seminar: How and why to determine structures in Inorganic Chemistry. The Importance of developing characterization strategies.

Contents of the Introduction Block:

Use of different characterization strategies both in solid state and in solution. Applications of the Elemental Quantitative analysis – C, H, N, S, O –, Quantitative analysis – ICP masses –, thermogravimetric analysis, molar ionic conductivity in solution, IR spectroscopy, Raman, Uv-V absorption spectroscopy, general mass spectrometry, NMR, RPE, RX diffraction – dust, monocrystal, etc –, and others.

Block 2. Vibrational Spectroscopy in Inorganic Chemistry

Block activities:

Lab Sessions:



- Propagation of the medium IR and/or distant IR spectra [VO (ACAC) 2] and [VO (ACAC) 2 (piperidine)]. Study of the displacement of the frequency ν ($\nu = \text{O}$) with the coordination of the N-donor ligand.

- Preparation of samples (KBR and Nujol-polyethylene tablets), generation and structural characterization of transition metal complexes: cis-[PtCl₂ (PPH₃)₂], Trans-[PtCl₂ (PPH₃)₂] and [PtCl₂ (DPPM)]

Seminar: introduction to the preparation of structural characterization strategies on the basis of two real practical cases in Inorganic Chemistry.

Contents of the vibrational spectroscopy block in Inorganic Chemistry:

Applications to the structural determination of inorganic compounds. Relation between binding forces and frequency displacement. Changes in the spectra of the ligands and transformation of the symmetry of the complex after coordination.

Block 3. Electronic spectroscopy in Inorganic Chemistry

Block activities:

Lab Sessions

- Realization of the Uv/Vis spectra of the complexes [Ni(NH₃)₆]Cl₂, [Ni(H₂O)₆]Cl₂ and [NET₄]₂[NiCl₄] and analysis of the resulting data. Importance of solvent.

- Observation of forbidden spin transitions and charge transfers: [Mn(H₂O)₆]²⁺ and [Fe(OX)₃]³⁻.

- Jahn-Teller effect observation: [Ti(H₂O)₆]³⁺

Contents of the electronic spectroscopy block in Inorganic Chemistry:

Types of electronic transitions in inorganic compounds and selection rules. Electronic spectra of octahedral and tetrahedral complexes. Diagrams of Orgel and Tanabe-Sugano. Covalency. Forbidden transitions. The spin-orbit coupling. Influence of the Jahn-teller effect. Other geometries. Charge Transfer (TC) spectra and intervalent...

Block 4. Mass spectrometry in Inorganic Chemistry

Block activities:

Seminar: Analysis of the use of different mass spectrometry techniques, taking as an example the PTA and 2-thiopyridine ligands, and some derivatives of Pd (ii) and Pt (ii) with these ligands.

Seminar: Analysis of the relationship between the structures of different transition metal complexes and information on their mass spectra.

Contents of the Block: Mass spectrometry in Inorganic Chemistry:

Different methods of ionization and analysis applicable to inorganic compounds (EI, FAB, MALDI, ESMS...). Relationship between structural information and the spectrum of masses that they present.

Block 5. Diffraction methods in Inorganic Chemistry

Block activities:

Seminar: Utilization of Crystallographic databases (CCDB).

Seminar: Symmetry of crystals. Space groups.

RX Diffraction Lab Session:

- Sample preparation: powder and growth of monocrystals

Seminar: Interpretation of data tables and diffraction patterns, both of monocrystal and of dust.

Contents of the Block: Diffraction methods in Inorganic Chemistry:

Solid-state symmetry elements. Space groups and cell representation unit. The diffractometer, RX interaction with the stuff and Bragg's law. RX diffraction on Monocrystal: stages in the resolution of a crystalline structure, structural information and crystallographic parameters.

Block 6. Nuclear magnetic resonance in Inorganic Chemistry (I)

Block activities:

Basic NMR Laboratory session in Inorganic Chemistry:

- Preparation and recording of ^1H , ^{31}P and ^{13}C NMR spectra of the complexes: CIS-[PtCl₂ (PPH₃)₂], trans-[PtCl₂ (PPH₃)₂] and [PtCl₂ (DPPM)]
- Structural determination of transition metal complexes: (II) complexes with different Schiff bases.

Seminar: Discussion of results of previous experiments IR + NMR.

Contents of the Block: Nuclear magnetic resonance in Inorganic Chemistry (I):

Active nuclei in NMR of interest in Inorganic Chemistry. Relevant information obtained from chemical displacement (from proton and other elements). Relevant information obtained from the relative intensity of the NMR signals. Simple spin systems due to coupling: homonuclear coupling and heteronuclear coupling. Coupling to nuclei with the quadrupole moment.

Relevant information obtained from the values of the coupling constants.

Block 7. Nuclear magnetic resonance in Inorganic Chemistry (II)

Block activities:

Advanced MRI Classroom session in Inorganic Chemistry:

- Examples of dynamic NMR of transition metal complexes.
- Examples of bi-dimensional NMR of transition metal complexes.

Seminar: Discussion of advanced NMR case studies.

Seminar: Solution of advanced NMR problems.

Contents of the Block: Nuclear magnetic resonance in Inorganic Chemistry (II):

More complex spectra (second order spectra; chiral inequivalence and Pro-chiral). The multinuclear approach. Relaxation (phenomena and experiments). Multiple resonance experiments: double resonance and triple resonance. The NOE effect. Pulse techniques. Monitoring of reactions: measurement of concentration and exchange reactions. Monitoring of dynamic processes by means of NMR.

Paramagnetic compounds.

Block 8. Structural characterization Strategies in Inorganic Chemistry

Block activities:

Seminar: Characterization Strategies Study: How to extract relevant information and how to avoid redundant information.

Tutoring: Individual solving of case studies with the preparation of a report.

5292 CHEMICAL ENGINEERING (II)

Single Topic Unit

TOPIC 1. Introduction

Introduction to the chemistry of transition elements. Transition elements in the periodic table: elements of Block D, elements of Group 12 and elements of Block F. Definition and characteristics of the elements of Blocks D and F. Trends of the transition elements.

TOPIC 2. Group 4: Ti, Zr and Hf.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Piezoelectric effect of BaTiO₃. Sulfides. Halides. Complex. Ziegler-Natta catalysts in the polymerization of olefins. Sharpless catalysts in the enantioselective epoxidation of olefins.

TOPIC 3. Group 5: V, Nb and Ta.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, trends and chemical reactivity, and applications. Oxides. Sulfides. Oxyanion and Polyoxometalate salts (POM). Halides. Complexes. Essentiality of V in some living organisms.

TOPIC 5. Group 7: Mn, Tc and Re.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Oxyanions. Halides. Complex. Role of Mn in photosynthesis (photosystem II). Use of ^{99m}Tc in Radiodiagnosis.

TOPIC 4. Group 6: Cr, Mo and W.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, trends and chemical reactivity, and applications. Oxides. Isopoly- and Hetero-poly anions (POM).

Bronzes of Mo and W. sulfides. Chevrel phases. Halides. Complexes. Multiple metal-metal bonds: Cr (II) acetate and quintuple m-m bonds Biological aspects of Cr and Mo.

TOPIC 6. Group 8: Fe, Ru and Os.



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General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, trends and chemical reactivity, and applications. Oxides. Oxyanions. Halides. Complexes. Prussian Blue. Biological aspects of iron.

TOPIC 7. Group 9: Co, Rh and Ir.

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, trends and chemical reactivity, and applications. Oxides. Sulfides. Halides. Complexes. The Knowles and Noyori catalysts in enantioselective hydrogenation processes: synthesis of L-DOPA and naproxen.

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General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, obtaining, physical properties, trends and chemical reactivity, and applications. Oxides. Sulfides. Halides. Complexes. Cyclic polymerization of Reppe. Wacker process. Monsanto and Cativa processes. CO-Detectors based on PdCl₂. Cytotoxicity of Pt compounds.

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General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, procurement, steelmaking and steels, physical properties, trends and chemical reactivity, and applications. Oxides. Sulfides. Halides. Complex. Ag halides in photography. Blue copper proteins in redox-type biological processes.

TOPIC 10. Group 3: Sc, Y, La and Ac, Lanthanides and actinide

General aspects of the elements: historical introduction, abundance and distribution, ores and minerals, extraction, physical properties, tendencies and chemical reactivity, and applications. Most important compounds.

5293 ADVANCED INSTRUMENTAL ANALYSIS

Advanced Instrumental Analysis

TOPIC 1. SENSORS

- Signal specificity in Instrumental analysis.
- Sensor concept.
- Optical sensors.
- Electrochemical sensors.



TOPIC 2. AUTOMATION IN INSTRUMENTAL TECHNIQUES

- Fundamentals of automation. Classification of methods.
- Techniques in segmented and non-segmented flow.

TOPIC 3. MASS SPECTROMETRY

- Fundamentals and generalities of instrumentation.
- Injection, ionization (electronics, chemistry, Plasma, MALDI, etc).
- Field analyzers, flight time, quadrupole, etc. Resolution. Detection.
- Coupling of chromatographic techniques.

TOPIC 4. METHODS BASED ON INDUCTION-COUPLED PLASMA SOURCES

- Induction-coupled plasma source (ICP).
- Optical emission spectroscopy with inductively coupled plasma (ICP-OES).
- Mass spectroscopy with inductively coupled plasma (ICP-MS).

TOPIC 5. THERMAL ANALYSIS METHODS

- Thermogravimetric analysis.
- Differential thermal analysis.
- Differential scanning calorimetry.
- Microthermic analysis.

TOPIC 6. X-RAY BASED METHODS

- Fundamental principles of X-rays. Instrumentation.
- X-ray absorption methods.
- X-ray diffraction methods.
- X-ray fluorescence methods.

TOPIC 7. SURFACE ANALYSIS

- Introduction to the study of surfaces in solids.
- Microscopy techniques for superficial analysis.
- Spectroscopic techniques of superficial characterization.

➤ **4th year**

5294 MATERIALS SCIENCE

MODULE I: MATERIAL PHYSICS

1. Structural and mechanical properties

Crystalline materials. Reciprocal network. Quasicrystals. Polycrystalline materials.
Amorphous materials. Nanomaterials. Elastic deformation. Modulus of elasticity and Shear. Plastic deformation. Punctual defects. Dislocations. Diffusion.

2. Vibrational modes and thermal properties

Mono and diatomic linear chain. Optical and acoustic modes. Phonons. Calorific capacity. Thermal conductivity. Thermal dilation.

3. Electronic and Magnetic properties

Band theory. Electrical conductivity. Semiconductor. Union P-N: Applications. Superconductivity. Paramagnetism and Diamagnetism. Ferromagnetism and Antiferromagnetism.

4. Optical properties

Absorption in metals and dielectrics. Reflectivity. Refraction. Dispersion. Polarization. Birefringence. Color. Optical fibers. Lasers. Non-linear optics.

5. Experimental and computational techniques

Diffraction. Optical, electron, tunnel and force microscopy. Surface techniques. Simulation of materials.

MODULE II: INORGANIC MATERIALS

6. Metallic materials and alloys

Homogeneous alloys and mixtures. Common alloys: Brass and bronzes. Light alloys. Special alloys. Iron-carbon alloys. Steels and Foundries.

7. Ceramic materials

Glasses. Structural ceramics and porcelain. Carbides, Nitrides and Borides. Ceramic Advanced. Refractory compounds. Abrasive materials. Zeolites. Cements.

8. Composite materials

Fiber-reinforced composite materials. Composite materials reinforced by particles. Laminated materials and sandwich structures. New ceramic and metal matrix composites.

9. Materials in the electronics industry

Devices. Superconductors, thermistors and varistors. Dielectric materials, ferroelectric and piezoelectric. Ionic conductors. Electrochromic materials. Liquid crystals.

10. Magnetic and optical materials

Hard and soft magnetic materials. Magnet applications. Storage of information. Optical materials. Applications.

MODULE III: ORGANIC MATERIALS

11. Concepts and definitions in Macromolecular Chemistry.

Introduction. Molecular weight and distribution of molecular weights in polymers. The solid state in polymers.

12. Polymerization methods and techniques.

Polymerization by steps. PCR. General Techniques of Polymerization.

13. Structure, properties and applications of polymers.

Polymers for general use. Engineering polymers and special polymers. Elastomers for general use.

5295 PROJECTS IN CHEMISTRY

Basic Project Theory

Topic 1. Project Basics

- 1.1. Project Definition.
- 1.2. Classification of project types.
- 1.3. Basic Features.
- 1.4. Project Management.

Topic 2. Project life-cycle

- 2.1. Characteristics of the project life-cycle.
- 2.2. Characteristics of the phases of the project.
- 2.3. Relations between project and product life-cycles.

Topic 3. Viability

- 3.1. Opportunity and need.
- 3.2. Current status of the subject matter.
- 3.3. Analysis and forecasting.

Topic 4. Management processes

- 4.1. Initiation.
- 4.2. Design and planning.
- 4.3. Implementation.
- 4.4. Control.
- 4.5. Closing.

Topic 5. Management areas in the planning and development of a project

- 5.1. Integration.
- 5.2. Scope.
- 5.3. Time.

- 5.4. Cost.
- 5.5. Quality.
- 5.6. Human Resources.
- 5.7. Communication.
- 5.8. Risk.
- 5.9. Acquisition.

Industrial Projects

Topic 6. Industrial Projects

- 6.1. Economy and industrial organization.
- 6.2. Process and product engineering.
- 6.3. Instrumentation and control of industrial processes.
- 6.4. Types of industrial projects.
- 6.5. Development of a particular case.

6294 MULTIVARIATE METHODS AND PROCESS ANALYTICAL TECHNOLOGY

MULTIVARIATE MODELS IN THE PAT INTRODUCTION TO MULTIVARIATE MODELING

The order of the signal. Models based on zero-order signals: model limitations based on single order signals: possibility of calibrating known interferences. Models based on two or higher order signals: possibility of calibrating in the presence of unknown interferences.

MODELS BASED ON MAJOR COMPONENTS

Multilinear regression by least squares. Soft model concept. Need for these models when there is correlation and/or collinearity in the data. Models based on minimum quadratic regression techniques on principal components (PCReg). Pretreatment. Choosing the correct number of components. Interpretation of the principal components. Construction of predictive models. Need for these calibrated in the determination of multicomponent mixtures with non-specific signals. Regression applications on major components in industrial problems. Practice: Simultaneous determination of food colorants contained in foods using UV-visible spectroscopy and calibration on principal components

MODELS BASED ON PARTIAL LEAST SQUARES

Regression adjustment criterion in partial least squares (PLS). Pretreatment: Centered, self-scaling, derivatives, SNV. Application of pre-treatment to different types of instrumental signals (NIR, fluorescence, UV-vis). Choice of the latent



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variables. Cross-validation. Predictive capacity of the PLS models. Possibility of detecting anomalous data: Q and T2 indexes. Power of the original variables. Application of PLS models in multivariate calibrations with overlapping signals. Interference modeling. Applications in polarography, voltammetry, molecular spectroscopy in UV-visible, molecular fluorescence, NIR and MIR spectroscopy, mass spectrometry.

Industrial applications of PLS.

Practice 1: Determination of a mixture of three commercial pharmaceutical drugs through UV-visible spectroscopy and PLS calibration.

Practice 2: Determination of moisture and protein in forages by spectroscopy NIR and calibration PLS. Effect of different pretreatments (derivatives, SNV) on the Merit figures obtained with the PLS model.

ON-LINE DETERMINATIONS

Need to adapt instrumental techniques to extract and to manage physico-chemical "on-line" information. Advantages and disadvantages. On-line spectroscopic type (UV-vis and NIR) measuring systems, chromatographic measuring systems and flow-injection analysis.

MULTIVARIATE PROCESS CONTROL

Multivariate nature of quality.

Definition of the final quality of a product

Characteristics of the process data and signal order. Analysis of a process and its practical operation, use of latent variables.

Advantage of multivariate control over the use of multiple univariate controls.

Industrial modeling and optimization, according to the recent proposals of the FDA on Analytical Process Technology (PAT) and the Harmonized Protocol (on "Quality by design " and design spaces, DS) to ensure product quality.

6295 INTRODUCTION TO NANOTECHNOLOGY

1. INTRODUCTION.

The nanoscale. Size-dependent properties. History of Nanoscience and Nanotechnology.

2. PROPERTIES OF NANOSTRUCTURES.

Mechanical, thermal and surface properties. Characteristic quantum phenomena. Confinement. Electronic, optical, magnetic and transport properties.

3. NANOSYSTEMS AND NANODEVICES.

Electronic. Magnetic. Photonic. Nano-electro-mechanical systems. Nanolayers.

4. QUANTUM TECHNOLOGIES.

Communication. Simulators. Sensors. Computers.

5. MATERIALS ON THE NANOSCALE.

Types of nanostructures. Carbon nanostructures. Metal nanostructures.
Non-metallic nanostructures.

6. NANOFABRICATION.

Bottom-up approximation. Top-down approximation.

7. CHARACTERIZATION OF NANOMETRIC MATERIALS.

Microscopy techniques. Superficial analysis techniques. Spectroscopic techniques.
Other techniques.

8. APPLICATIONS AND SOCIAL IMPACT OF NANOTECHNOLOGY.

Scientific, medical and industrial applications. In what direction is Nanotechnology going? Impact of nanotechnology on society.

6296 RENEWABLE ENERGIES

Unit 1. General aspects

TOPIC 1: Energy, environment and sustainability.

TOPIC 2: Sources, resources and energy reserves.

TOPIC 2. Non-renewable energies

TOPIC 3: Non-renewable resources and transformation processes.

TOPIC 4: Classical thermoelectric power plants and nuclear power plants.

Unit 3. Renewable Energies

TOPIC 5: Solar radiation.

TOPIC 6: photothermic Solar energies and photovoltaic solar energy. Its conversion

TOPIC 7: Wind power.

TOPIC 8: Hydraulic power.

TOPIC 9: Other energies. Sea power, geothermal, biomass.

TOPIC 10: Present and future of renewable energies. Energy storage.
Sustainability.

Unit 4. Environmental Effects of energy utilization

TOPIC 11: Pollution and ecosystems.

TOPIC 12: Environmental effects of different energies.

Unit 5. Practical Experiences

TOPIC 13: Practical Experiences.

6297 PERSPECTIVES IN ORGANIC CHEMISTRY

Advanced Organic Synthesis

Anions stabilized in organic synthesis

Enolates and their application in the formation of carbon-carbon bonds. Study of the stereochemistry of the reactions

Reactive intermediates in organic synthesis

Description of reactive intermediates: carbocations, carbenes, nitrenes and radicals. Applications in organic synthesis

Introduction to total synthesis and retrosynthetic analysis

Resolution of problems based on total synthesis using retrosynthetic approximation.

Structural elucidation of organic compounds

Nuclear Magnetic resonance

Basics. NMR of ^1H and ^{13}C in the elucidation of organic compounds. Introduction to two-dimensional experiments.

6298 ENVIRONMENTAL CHEMISTRY

Block I: Environmental chemistry of the atmosphere

- Terrestrial atmosphere, phenomena in the outer atmospheric layers.
- Chemical and photochemical reactions in the atmosphere.
- Atmospheric oxygen reactions.
- Atmospheric nitrogen reactions.
- Air pollution: particle effects.
- Polluting effect of sulfur dioxide.
- Photochemical smog.
- Acid rain.
- Destruction of the ozone layer.

Block II: Environmental chemistry of the hydrosphere

- Water, important properties.
- Chemical processes of water.
- Gases in the water.
- Acidity and CO_2 in the water. Alkalinity.
- Complexes and Chelates.
- Oxidation-reduction reactions in water.
- Colloidal particles in the water. Formation of sediments.
- Bacterial metabolisms: microbial transformations.
- Water pollution: nature and types.
- Water treatment and use. Reuse and recycling.

Block III: Environmental chemistry of the lithosphere

- Nature of solids in the lithosphere.
- Environmental aspects in the lithosphere.
- Soil and food production: fertilizers, nutrients, pesticides, waste and soil contaminants.
- Environmental chemistry of terrestrial systems: industrial ecology.
- Green chemistry and industrial ecology for the prevention and treatment of waste.
- Environmental chemistry of the biosphere and toxicological chemistry.
- Environmental Chemical Analysis.

6299 ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

UNIT I: ORGANOMETALLIC CHEMISTRY

TOPIC 1: Introduction.

Definitions. Historical development of Organometallic Chemistry. Types of links and relation with the periodic table. General properties of compounds. Organometallic. Stability and reactivity of the M-C bonds.

TOPIC 2: Organometallic compounds of the elements of the S and P groups.

Organometallic of alkaline Metals. Metal organometallic compounds. Alkaline. Organometallic of Zn, Cd and Hg. Carboranes, Metalloboranes, Organo-aluminates and organometallic compounds of Ga, In and Tl. Organosilicon compounds, germanium, tin and lead.

TOPIC 3: Organometallic compounds of transition elements

General points

Transition elements. Electronegativity and Bond strength. Types of ligands. Types of complexes. Rule of the 16/18 electrons. Oxidation state and counting Electrons.

TOPIC 4: Organometallic complexes of transition elements with Sigma Metal-Carbon bonds

Alkyl transition complexes. β -elimination of hydrogen. Complexes with agostic bonds. Synthesis of transition metal alkyls. Alkynyl compounds. Reactivity of transition metal alkyls.

TOPIC 5: Organometallic compounds with carbon-bonded π -acid ligands

Ligands with π retrodonation. Carbonyls of transition metals. Isoelectronic ligand bonding to carbonyl. Alkylidene and alkylidene complexes: the M-carbene bond,

Fischer and Schrock Carbenes, synthesis of carbene complexes, reactivity of carbene complexes, synthesis of carbene complexes, reactivity of carbene complexes. Organometallic complexes with π -donor ligands: alkene and dien, alkyl, alkyne, cyclopentadienyl, arene compounds.

UNIT II: BIOINORGANIC CHEMISTRY

TOPIC 6: Inorganic elements in biological systems.

Biological functions of elements and inorganic compounds. Minerals. Bioavailability of inorganic elements. Recruitment and transformation of the trace elements. Metal-protein interactions: entatic state. Study with models.

TOPIC 7: Bioinorganic Chemistry of alkali metals and alkaline earth metals.

Cell membrane. Transport of cations through the membranes. Biological functions of calcium. Biological functions of magnesium.

TOPIC 8: Bioinorganic Chemistry of iron and copper.

BLOCK I (IRON): Hemoproteins. Proteins Fe/S. Proteins that contain Fe-O-Fe units. Iron metabolism. BLOCK II (COPPER): Copper oxidases. Electron-transporting copper proteins. Oxygen-carrying copper proteins. Copper monooxygenases. Superoxide dismutase of copper and zinc. Copper metabolism.

TOPIC 9: Bioinorganic Chemistry of zinc, molybdenum and cobalt.

BLOCK I (ZINC): Carbonic anhydrase. Hydrolases. Dehydrogenases. Dehydratases and polymerases. "Fingers" of zinc. Zinc metabolism. BLOCK II (MOLYBDENUM): Molybdenum cofactor-dependent enzymes. Molybdenum and iron cofactor dependent enzymes. Molybdenum metabolism. BLOCK III (COBALT): Vitamin B12. Biological behavior of the cobalamins. Glucose-isomerase. Cobalt metabolism.

TOPIC 10: Bioinorganic Chemistry of other transition metals and non-metallic elements.

BLOCK I (OTHER TRANSITION METALS): Vanadium. Chrome. Manganese. Nickel. BLOCK II (NON-METALS): Halogens. Selenium. Arsenic. Silicon. Oxygen.

TOPIC 11: Pollution and Toxicology. Applications in medicine and pharmacology.

BLOCK I (CONTAMINATION AND TOXICOLOGY): Toxicity mechanisms. Defense and detoxification mechanisms. Toxicity of metal elements. Toxicity of radioactive elements. Toxicity of non-metallic elements. Acid rain. Ozone layer. BLOCK II (MEDICAL APPLICATIONS AND PHARMACOLOGY): Chelation therapies. Supplementation of essential elements. Metal complexes with anti-tumor activity. Other applications.

6300 SOFTWARE TOOLS IN CHEMISTRY

2D Representation

2D Molecular Representations

Drawing of simple molecules. Drawing of aromatic systems. Drawing of molecules with stereocentres. 3d drawing. Advanced templates and drawing tools.

NMR spectrum processing

Single-dimensional NMR spectra

IDF FT processing. Phase adjustment. Baseline adjustment. Referenced. Integration.

Two-dimensional NMR spectra.

Two-dimensional NMR spectrum processing. Phase adjustment. Analysis of the two Phases of the spectrum.

Molecular structural aspects

Cambridge Structural Database

Introduction to the ConQuest system. Elementary searches. Advanced searches. Analysis of structural data.

Data processing in chemistry

Spreadsheets. Symbolic and numerical calculus programs

Data analysis. Regressions. Representations of two-dimensional data diagrams. Data representations in three-dimensional diagrams. Operating useful software for analyzing data in chemistry: EXCEL, MATLAB, MAPLE, GNUPLOT.

6301 CHEMISTRY APPLIED TO LIFE SCIENCES

Structure of biomolecules

Topic 1: Structure and conformational analysis of biomolecules

Protein structure. Basic conformational problems of proteins. General characteristics of the nucleic acid structure. Stabilizing forces of ordered nucleic acids. Structure of other biological polymers.

Techniques for the study of biomolecules

Topic 2: Spectroscopic and diffraction techniques

Protein and nucleic acid absorption spectroscopy. Optical rotary dispersion and dichroism of biological molecules. Protein emission spectroscopies and nucleic acids. Application of infrared and Raman spectroscopies. Nuclear magnetic resonance interactions. Paramagnetic resonance of the biomolecule electron. Determination of the protein structure by X-ray crystallography. Comparison of X-ray crystallography with multi-dimensional NMR. Structural databases.

Topic 3: Methods for the separation and characterization of biomacromolecules

Ultracentrifugation. Rotational viscometry. Electrophoresis. Mass spectrometry.



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Application of techniques for the analysis of biological macromolecules

Topic 4: Interaction of biopolymers with ligands and conformational equilibrium of biomolecules

Interaction of proteins with ligands. Interlayers in nucleic acids. Helix-coil transition in proteins. Reversible protein folding. Transitions. Structural nucleic acid. Introduction to biological membranes.