

## Study programme: Chemistry and Technology

### Specialization: Chemistry

The exam comprises 3 topic areas selected from the following:

1. **Inorganic Chemistry** (based on General and Inorganic Chemistry I and II)
2. **Organic Chemistry** (based on Organic Chemistry I and II)
3. **Physical Chemistry** (based on Physical Chemistry I and pre-requisites thereof)
4. **Analytical Chemistry** (based on Analytical Chemistry I and pre-requisites thereof)

### Selection of topic areas according to the focus of the thesis

- The topic areas 1 and 2 are compulsory for all students.
- Student chooses elective topic area 3 or 4 according to his preference. The choice should be declared before the submission of the thesis at the office of supervisor's department

#### Topic area „Inorganic Chemistry“

1. Atomic structure, electronic structure of atoms, atomic orbitals; periodic system, effective charge of atomic nuclei and its influence on periodic trends in physical-chemical properties of elements.
2. Chemical bonding - bond types, energy character of inter- and intramolecular bonds; physical properties predictable using type of bonding.
3. Molecular Orbitals Theory – bonding in diatomic molecules, bond order, and magnetism of molecules.
4. Valence Bond Theory; hybridization, Lewis structures, VSEPR; physical properties of molecules, molecular symmetry.
5. Lewis acid-base theory and its implications in inorganic chemistry; mechanisms of LA/LB reactions.
6. Acid-base theory; acid-base reactivity, simple ions and oxoanions in aqueous solutions, hydrolysis, solubility of salts; diagrams of predominant forms.
7. Coordination complexes; coordination bonding, ligand field splitting of d-orbitals; bonding types of ligands; structural isomerism and stereoisomerism.
8. Principles of redox reactions, reducing and oxidizing agents; standard reduction potentials; fundamentals of electrochemistry; Pourbaix diagrams.
9. Ionic bonding; structure and symmetry of crystalline solids; reactivity and properties of solid hydrides, halides, oxides, and other binary compounds of metals and p-elements.
10. Metallic bonding; trends in physical properties of metals; redox reactivity of metallic elements; production of important metals.

#### Topic area „Organic Chemistry“

1. Alkanes and alkenes, radical and electrophilic addition, oxidation and reduction.
2. Alkynes and dienes, single and double electrophilic addition to alkynes, acidity of terminal alkynes, 1,2- and 1,4-addition to dienes, Diels-Alder reaction.
3. Arenes, electrophilic and nucleophilic substitution of arenes and heteroarenes, role of directing substituents, diazotization and reactions of diazonium salts, oxidation and reduction.
4. Haloalkanes – bimolecular and monomolecular nucleophilic substitution and elimination.
5. Alcohols and phenols, bimolecular and monomolecular nucleophilic substitution, oxidation and reductions, transformation to alkyl alkan- and arenesulfonates and their reactions.
6. Organometals, preparation and reactions; ethers including oxirane, preparation, applications and reactions.
7. Aldehydes and ketones, nucleophilic addition, oxidation and reduction.
8. Carboxylic acid and non-nitrogen functional derivatives of carboxylic acids – acyl halides, anhydrides and esters, acyclic (tetrahedral) nucleophilic substitution, reduction.

9. Reactions of enols and enolates, halogenation of aldehydes and ketones, aldol and Claisen condensation, acetoacetic and malonester synthesis.
10. Nitrogen containing compounds – amines; nitrogen functional derivatives of carboxylic acid – amides and nitriles and their reactions, acyclic nucleophilic substitution of amides, reduction.
11. Heterocumulenes,  $\alpha,\beta$ -unsaturated oxo compounds, carbonic acid derivatives.
12. Heterocycles, basic types of five- and six-membered heterocycles, aromaticity. Basicity, reactions on nitrogen, electrophilic and nucleophilic substitution reactions.
13. Amino acids and peptides, synthesis of coded amino acids, protection of terminal C- and N- groups of amino acids, peptide synthesis and analysis.
14. Saccharides, structure, stereochemistry, configuration, cyclic forms, oxidation and reduction, glycosides, reducing and non-reducing disaccharides, polysaccharides). Structure of nucleic acids, principles of base pairing.

#### Topic area „Physical Chemistry”

1. State behaviour of gases. The ideal gas equation, the van der Waals equation, critical properties of pure substances.
2. The first law of thermodynamics. Internal energy, enthalpy, work, heat, adiabatic processes.
3. The second and third laws of thermodynamics. Entropy, Gibbs and Helmholtz energies.
4. Thermochemistry. Heat capacities, reaction heat, the Hess' law and Kirchhoff's laws.
5. Thermodynamic description of mixtures. Partial molar quantities, excess functions, chemical potential, activity, standard states.
6. The Gibb's phase rule. Phase equilibrium of one-component systems. Clapeyron equation, Clausius-Clapeyron equation, phase diagrams.
7. Vapour-liquid and gas-liquid phase equilibria. The Rault's and Henry's laws, typical phase diagrams, azeotropes.
8. Liquid-liquid and solid-liquid equilibria. Typical phase diagrams, thermodynamic description of equilibria in two-component systems. The lever rule.
9. Chemical equilibrium of simple reactions. Equilibrium constant, mass balance, the response of equilibrium to the conditions.
10. Electrochemical processes. Electrolytic cells, the Faraday's law, galvanic cells, the Nernst equation, standard potentials.
11. Chemical kinetics of simple reactions. Rate laws, reaction order, rate constant and its temperature dependence, half-life of a reaction, integrated rate laws for reactions of zero, first, and second order.

#### Topic area „Analytical Chemistry“

1. Basic terms (sample, analyte, matrix, interferent, analytical signal, analytical process, sampling methods, quartering).
2. Volumetric analysis (basic concepts, divisions and principles of titrimetric methods, titration curve, equivalence point and its indication).
3. Gravimetric analysis (basic concepts, precipitation and weighing forms, gravimetric procedure).
4. Potentiometry, pH measurement (electrode types, electrode selectivity, direct potentiometry, potentiometric titration).
5. Dynamic electroanalytical methods (voltammetry, polarography, coulometry).
6. Gas and liquid chromatography (overview and principles of particular techniques, important parameters and quantities, detection methods, qualitative and quantitative analysis).
7. Lambert-Beer's law and its use (quantities, deviations from validity, application).
8. Spectrometric instrumentation (basic building blocks of emission, absorption and fluorescence spectrometers).
9. Atomic spectrometry (overview and principles of individual techniques).

10. Molecular spectrometry (overview and principles of individual techniques).
11. Mass spectrometry (basic building blocks of mass spectrometer, ionization and ion separation techniques, application in qualitative and quantitative analysis).
12. Calibration methods (calibration curve method, standard addition method, internal standard method) and standards (chemical standard, reference material, certified reference material).