

Study programme: Chemistry and Technology

Specialization: Chemical Technology

The exam comprises 3 topic areas selected from the following:

1. **Chemistry and Chemical Technology** (based on General and Inorganic Chemistry I and II, Organic Chemistry I and II, Fundamentals of Chemical Technologies)
2. **Physical Chemistry** (based on Physical Chemistry I and pre-requisites thereof)
3. **Chemical Engineering** (based on Unit operations of Chemical Engineering I and II)
4. **Catalysis** (based on Catalysis, Applied Chemical Processes)

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 „Chemistry and Chemical Technology“

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; Molecular Orbitals Theory – bonding in diatomic molecules, bond order, magnetism of molecules.
3. Valence Bond Theory; hybridization, Lewis structures, VSEPR; physical properties of molecules, molecular symmetry; Lewis acid-base theory; mechanisms of LA/LB reactions.
4. Acid-base theory; acid-base reactivity, simple ions and oxoanions in aqueous solutions, hydrolysis, solubility of salts; diagrams of predominant forms.
5. Coordination complexes; coordination bonding, ligand field splitting of d-orbitals; bonding types of ligands; structural isomerism and stereoisomerism.
6. Principles of redox reactions, reducing and oxidizing agents; standard reduction potentials; fundamentals of electrochemistry; Pourbaix diagrams.
7. Ionic and metallic bonding; structure and symmetry of crystalline solids; reactivity and properties of metals and, solid binary compounds of metals and p-elements.
8. Non-aromatic hydrocarbons, alkanes, alkenes, alkynes and dienes - radical and electrophilic addition, oxidation and reduction, Diels-Alder reaction.
9. Arenes and heteroarenes - electrophilic and nucleophilic substitution of arenes and heteroarenes, role of directing substituents, diazotization and reactions of diazonium salts, oxidation and reduction.
10. Haloalkanes – bimolecular and monomolecular nucleophilic substitution and elimination, transformation to organometals and their reactions.
11. Alcohols and phenols – bimolecular and monomolecular nucleophilic substitution, oxidation and reductions, transformation to alkyl alkan- and arenesulfonates and their reactions; ethers – applications and reactions.
12. Aldehydes and ketones, nucleophilic addition, aldol condensation, oxidation and reduction, α,β -unsaturated oxo compounds, saccharides.
13. Carboxylic acid and non-nitrogen functional derivatives of carboxylic acids – acyl halides, anhydrides and esters, acyclic (tetrahedral) nucleophilic substitution, reduction, Claisen condensation, acetoacetic and malonester synthesis.
14. Nitrogen containing compounds – amines; nitrogen functional derivatives of carboxylic acid – amides and nitriles and their reactions, acyclic nucleophilic substitution of amides, reduction, heterocumulenes, amino acids and peptides.
15. Primary and secondary crude oil processing.
16. Petroleum chemistry (steam cracking, ethylene, propylene and benzene based processes).

17. Processing of natural gas, C1 chemistry.
18. Mineral acids production (sulphuric acid, nitric acid).
19. Ammonia production and fertilisers.
20. Electrochemical production of hydrogen, chlorine and caustic soda.

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 „Chemical Engineering“

1. Principles of material balances.
2. Principles of enthalpy balances in systems with and without a chemical reaction.
3. Flow in pipes, Bernoulli equation, continuity equation, pumps.
4. Cake filtration (kinetics of filtration, washing, filter press).
5. Settling and fluidization (terminal velocity of settling, threshold of fluidization, terminal velocity of fluidization).
6. Liquid-liquid extraction: single-stage extraction, repeated cross-flow extraction, counter-current extraction, immiscible solvent, partially miscible solvents.
7. Distillation - flash, batch, continuous with reflux (rectification).
8. Drying - properties of humid air, continuous drying, batch drying.
9. Absorption - staged, continuous contact of phases.
10. Chemical reactors - continuous stirred-tank reactor, batch reactor, tubular reactor, cascade of CSTRs.
11. Heat transfer (conduction, convection, overall heat transfer), heat exchangers.
12. Mass transfer (diffusion, convection, overall mass transfer).
13. Membrane processes - gas permeation, pervaporation, ultrafiltration, nanofiltration, reverse osmosis.

Topic area „Catalysis“

1. Principles of acceleration and directing chemical reactions by catalysts.
2. Solid catalysts. Model surfaces.
3. Adsorption in catalysis.
4. Catalyst characterization - temperature-programmed techniques, ion-spectroscopy, X-ray photoemission spectroscopy, Mössbauer spectroscopy, diffraction methods, methods of X-ray absorption, vibrational spectroscopy, microscopy).
5. Catalyst deactivation and reactivation.
6. Industrial catalytic processes - showcases of heterogeneous, homogeneous, and biocatalysis.
7. Environmental catalysis.
8. Material and energetic balance of the chemical process. Stoichiometry, conversion, excess and reaction enthalpy effect on the reaction system.
9. Chemical equilibria and ways how to change yield of the reaction in chemical technology.
10. Kinetics of the chemical reaction, methods of its variation in the industry.
11. Mass and heat transfer in the chemical reactors.
12. Separation processes and its role in the chemical technology.
13. Electrochemical reactors design basic components and its properties.
14. Electrochemical reaction, electrochemical potential, overvoltage, influence of overvoltage on final product.