RECRUITMENT

CHEMICAL SCIENCES

2023/2024

Doctoral School of Exact and Natural Sciences

CONTENTS

ABOUT THE SCHOOL

The main element of education at the Doctoral School of Exact and Natural Sciences (SDNSP) is the implementation of an individual PhD project in one of the scientific disciplines (Astronomy, Computer Science, Mathematics, Biological Sciences, Chemical Sciences, Physical Sciences, Earth and Environmental Sciences) that are covered by the school, under supervision of a faculty member chosen by the doctoral student.

The education at SDNSP lasts 4 years and includes courses in the form of specialization and monographic lectures, workshops, seminars, two-day symposiums as well as courses and trainings to improve the skills of doctoral students in teaching.

The graduate of the Doctoral School of Exact and Natural Sciences has a highly specialized education acquired under the supervision of leading scientists and is prepared to undertake independent scientific and teaching activities at universities and research institutes. In addition, the graduate gains extensive knowledge beyond the discipline in which he/she prepares his/her doctoral dissertation, as well as skills in conducting scientific and teaching activities.

ACADEMIC DISCIPLINES

biological sciences
limit of **17** places

astronomy
limit of **5** places

Earth and related environmental sciences
limit of **11** places

mathematics and computer sciences
limit of **22** places

chemical sciences
limit of **18** places

physical sciences
limit of **27** places

SCHOLARSHIP

In accordance with Art. 209 of the act of 20 July 2018 – The Law on Higher Education and Science, a doctoral student who does not hold a degree of doctor shall receive a doctoral scholarship. The total period of receiving the doctoral scholarship at doctoral schools shall not exceed 4 years. The amount of a monthly doctoral scholarship shall be at least: 37% of a professor's salary – up to the month in which the mid-term evaluation was conducted; 57% of a professor's salary – after the month in which the mid-term evaluation was conducted. The amount of the minimum basic salary of a professor is currently PLN 7210 gross. The above-mentioned amounts may change if the Ministry responsible for higher education and science decides to announce a new base a professor's salary.

Each doctoral student (who does not hold a degree of doctor) receives a scholarship in the amount not less than:

– PLN **2667.70*** gross for the first two years of studies (before the mid-term evaluation);

– PLN **4109.70*** gross in the next two years after the mid-term evaluation.

Supplement for people with disabilities: PLN 800.31

*The amounts shown are for doctoral students admitted in the limit recruitment.

SUPERVISOR

It is worth starting the recruitment process to a doctoral school at the University of Warsaw by finding a supervisor, who are willing to provide care for the doctoral student and perform scientific supervision over their research project. In order to find a supervisor, candidates for the Doctoral Schools are encouraged to search through the database of supervisors. The database contains the list of University of Warsaw researchers, who are willing to perform the function of the dissertation supervisor.

promotorzy.szkolydoktorskie.uw.edu.pl/en/search

Please note that not all potential supervisors are on the list. The candidates are also encouraged to consult the websites of the University of Warsaw faculties and academic units for the information on academic teachers conducting their research.

en.uw.edu.pl/about-university/faculties/

According to the School Regulations, a potential supervisor can only be a person with:

- the habilitated doctor (doktor habilitowany) degree or an equivalent degree or the title of professor as well as has to be an employee of the University of Warsaw or the employee of the institution co-running the School (Institute of Mathematics Polish Academy of Sciences);
- the status of retired professor at the University of Warsaw.

The dissertation supervisor can be a person, who remains a dissertation supervisor for no more than five doctoral students or persons applying for being awarded the doctor degree (e.g. participants of doctoral studies who have initiated a doctoral dissertation process). In exceptional instances, the Director of School may increase this limit.

RECRUITMENT SCHEDULE

8 May – 19 June 2023
registration in the system of Internet Recruitment for Candidate (IRK)

application for admission to the School, payment of the admission fee (PLN 200)

until 30 June 2023
sending recommendation letters

until 4 July 2023
publication of the interview schedule

4 July – 21 July 2023
qualification procedure

until 4 Aug. 2023
announcement of the ranking list

7 Aug. – 21 Sept. 2023
accepting documents from qualified candidates

until 30 Sept. 2023
announcement of the list of accepted candidates

October 2023 – beginning of education

HOW TO APPLY

1

See the admission requirements for the Doctoral School of Exact and Natural Sciences in the discipline of Chemical Sciences.

2

Register in the Internet Recruitment for Candidate (IRK) system: irk.uw.edu.pl

3

Complete your personal details and submit all the necessary documents.

4

Pay the admission fee to the individual account visible in the IRK system.

5

Check the Doctoral School's website for qualification examination and interview dates.

6

Take the exam and interview by the deadline.

7

Check the Doctoral School's website and the IRK system for the results of the qualification proceedings.

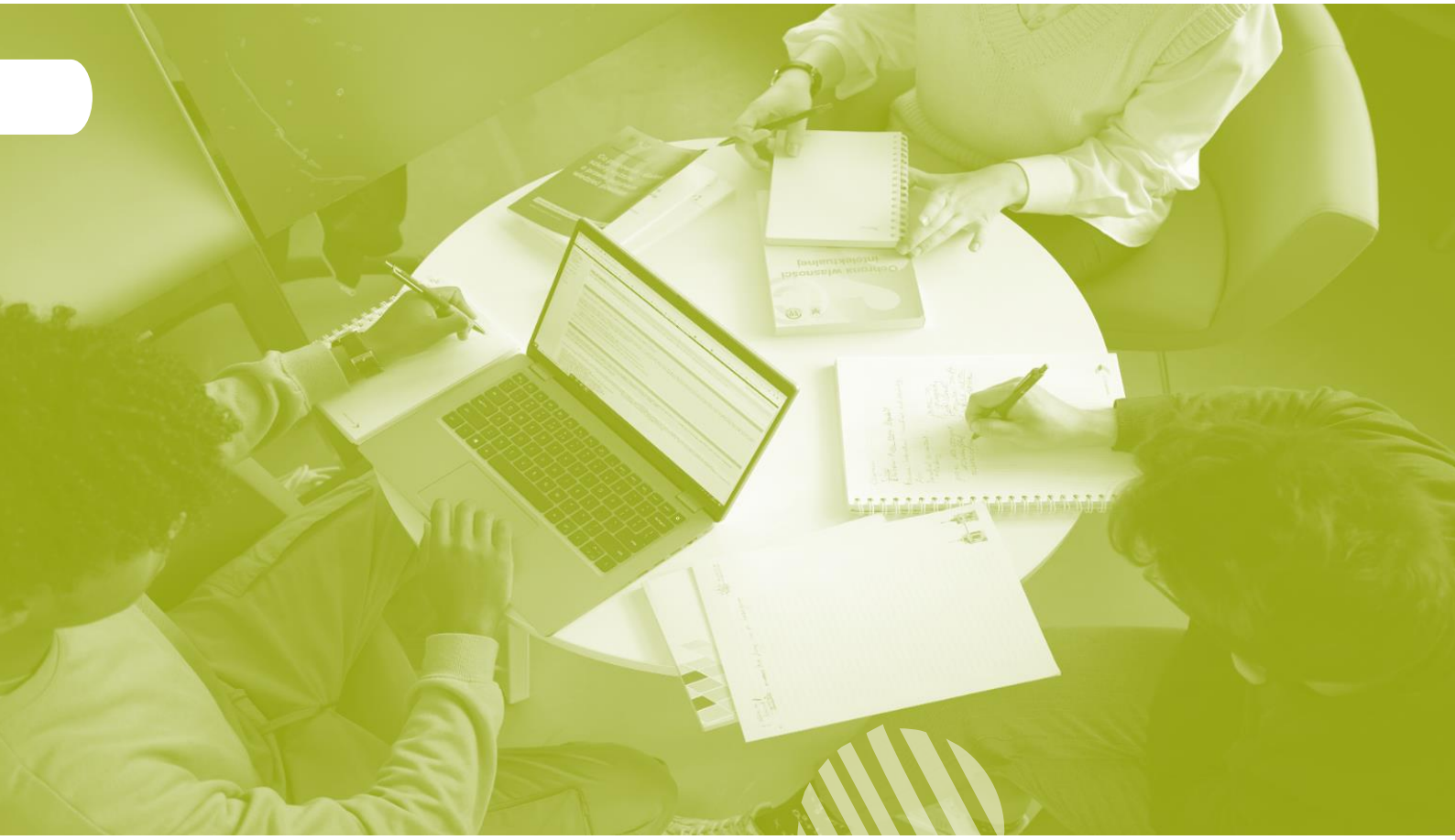
8

Submit the required documents to the office of the Doctoral School of Exact and Natural Sciences.

9

Once you have received information in the IRK system about your admission to the Doctoral School, follow the instructions provided by the office of the School.

REQUIRED DOCUMENTS



The candidate shall submit a School admission application only through the Internet Recruitment for Candidate (IRK). Once all required documents are attached in the system of IRK, pages are saved, and the fee is paid, no further steps need to be taken. The application is saved and does not need to be submitted.

THE APPLICATION SHALL INCLUDE

1

indication of the selected discipline in which the candidate plans to pursue education or in the case of applying for the Interdisciplinary Doctoral School – fields of science with the specification of the leading field (and where there is no leading field – at least two equivalent disciplines), PESEL number or passport number, nationality, contact information (residence address, e-mail address, telephone number), information whether the candidate agrees to receive administrative decisions by means of electronic communication, consent for processing of personal data for the purposes of the admissions procedure;

2

(applies to candidates holding a Master's degree or an equivalent degree obtained under separate regulations or, in accordance with their declaration, who shall hold such a degree by 21 September 2023) a scan of the graduation diploma of uniform master's degree or postgraduate studies or an equivalent diploma obtained under separate regulations, or in the case of candidates pursuing education in the European Higher Education Area – a certificate of holding a master's degree or a statement that the diploma or certificate confirming the award of a master's degree will be delivered by 21st of September 2023, in the case of a diploma equivalent to a uniform master's degree or postgraduate studies graduation diploma, a candidate shall justify such equivalence. In case the diploma was issued in a language other than Polish or English, the candidate shall attach its certified translation;

(applies to candidates who are a graduate of a first degree program or a students who have completed the third year of a unified master degree program, and have been approved by the Director in consultation with the qualification team to be considered for admission due to their exceptional, superior scientific achievements demonstrated so far) the candidate shall attach the Director's consent.

3

a description of the initial research project proposal in English; The description may not exceed four pages, font type: Times New Roman or equivalent, font size: at least 11 points, line spacing: 1, upper and lower margin: at least 1.5 cm, side margins: at least 2 cm, the references shall be include in the page limit;

4

a resume or CV outlining the candidate's scientific activity, including scholarly interests and achievements during the five calendar years preceding the application (if a candidate became a parent during this time, as evidenced by a scan of the child's birth certificate attached to the application, this period shall be extended by two years for each child), including, but not limited to:

- publications,
- research and organizational work at student research groups,
- participation in scientific conferences,
- participation in research projects,
- awards and honorable mentions,
- research internships,
- research skills training programs completed,
- activities promoting science,
- activity in science movement representative bodies,
- average of their university grades,
- professional career,
- level of proficiency in foreign languages;

5

scans of materials evidencing scientific activity mentioned in their CV and/or resume;

6

a document confirming at least B2 proficiency level in English or a declaration of the level of proficiency in English allowing education at the School;

7

the scan of a declaration by the planned supervisor, confirming their agreement to undertake the duties of a supervisor and of the number of doctoral students, for whom they perform the duties a designated supervisor, in accordance with the template constituting Appendix no.4 to the Resolution no. 17 of the Senate of the University of Warsaw of 20th January 2021 on rules of admission to doctoral schools at the University of Warsaw (the University of Warsaw Monitor of 2021, item 142), the candidate may also attach a scan of their planned supervisor's opinion and opinions of other academics about the candidate and their scientific activity and/or proposed research project;

8

the photograph of a candidate's face that allows for their identification;

9

a declaration confirming whether the candidate was or is a doctoral student or a participant of doctoral studies or whether they have initiated a doctoral dissertation process or whether proceedings to award them a doctoral degree have been initiated – and if yes, the title of their doctoral dissertation or the research project prepared by a candidate, including the name and last name of the candidate's tutor or supervisor;

10

a declaration confirming that they have reviewed the Resolution no. 17 of the Senate of the University of Warsaw of 20 January 2021 on rules of admission to doctoral schools at the University of Warsaw (the University of Warsaw Monitor of 2021, item 142) and Articles 40 and 41 of the Code of Administrative Procedure;

11

abstract of the master's thesis or master's project in English (up to 3,000 characters with spaces);

12

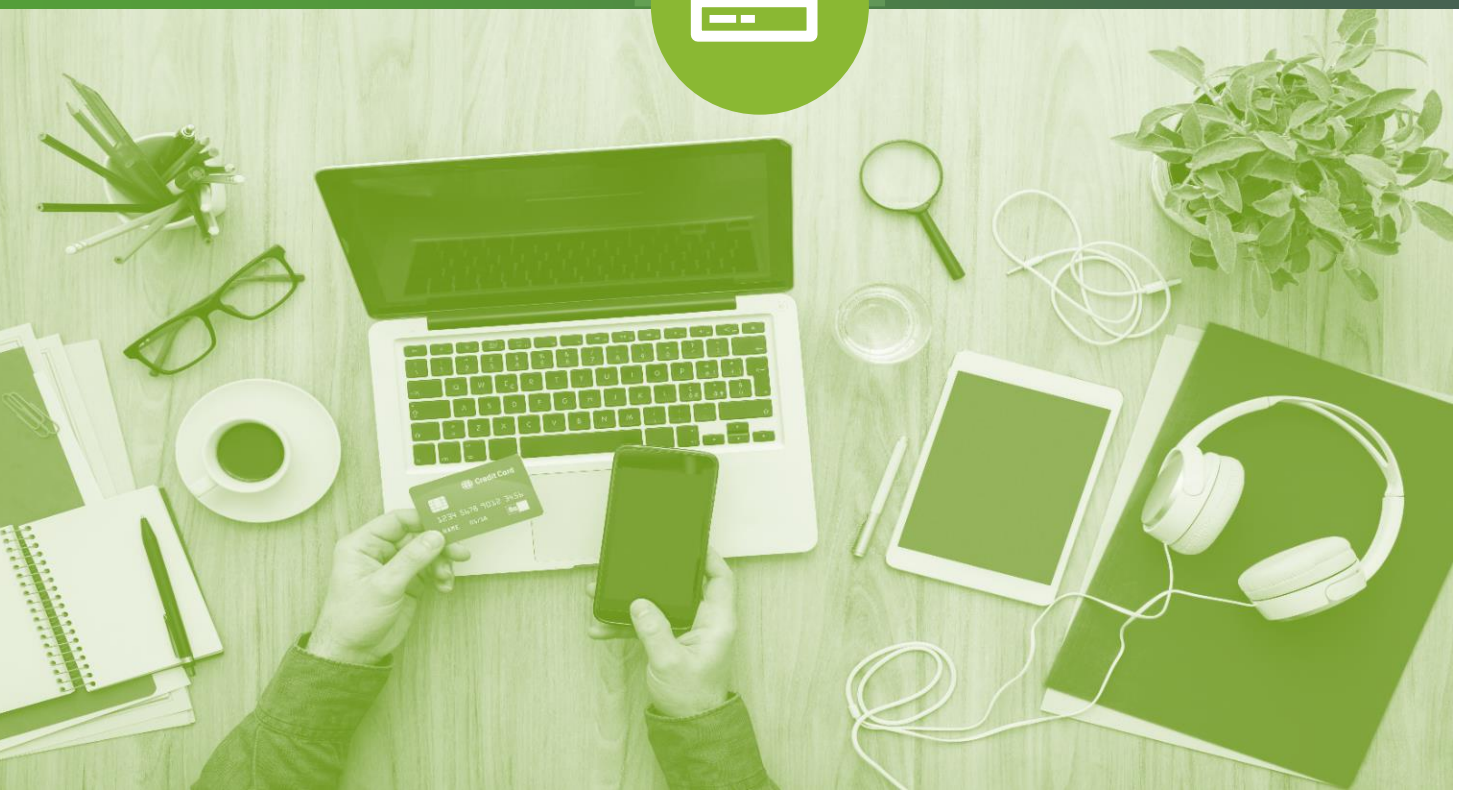
scanned transcripts of records of the graduate and postgraduate studies or the uniform Master's degree studies, or equivalent documents (e.g. diploma supplement);

13

contact data of two persons who will send recommendation letters regarding the candidate directly to the address **sd.nsp.chem@uw.edu.pl**, which is specific for a given disciplines. It is the candidate's responsibility to ensure that the person who makes the recommendation sends the letter. A failure of receiving the recommendation letters does not mean that the application for admission to the School is incomplete; the letters may be taken into consideration when evaluating the candidate's scientific potential;

RECRUITMENT FEE

The recruitment fee is PLN 200 and is paid to the candidate's individual account generated in the IRK system.



INSTRUCTION FOR COMPLETING THE APPLICATION FOR ADMISSION TO THE SDNSP

In order to complete the application for admission to the Doctoral School of Exact and Natural Sciences correctly, there have been the instructions published on the School's website, which may be helpful when registering in the **Internet Recruitment of Candidates** (IRK) system.

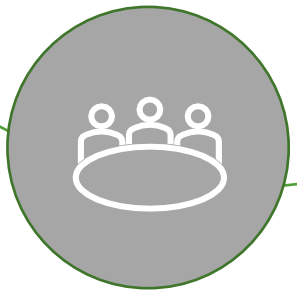
QUALIFICATION PROCEDURE

one-stage procedure

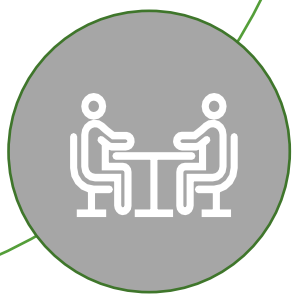
initial research project proposal
5 points

100
points

scientific activity of the candidate
15 points



qualification examination
40 points



interview
40 points

ASSESSMENT CRITERIA AND METHODS

5 points

Initial research project proposal

When evaluating the initial research project proposal, the following shall be taken into account:
1) the feasibility of the project in the context of documented competencies of the candidate;
2) the academic importance of the project;
3) anticipated added value for the scientific community of the academic discipline.

15 points

Scientific activity of the candidate

When evaluating scientific activity, the following elements, confirmed by means of scanned documents, shall be taken into account:
1) scientific publications (a scan of the front page is required; in the case of multi-author achievements, the percentage share of the candidate's participation in the achievement must be defined)
2) confirmed participation in student competitions;
3) confirmed participation in research projects (a scan of the certificate issued by the project coordinator is required);
4) presentations delivered or seminar and conference messages (a scan confirming presentation delivery is required);
5) documented research internships;
6) achievements within students' research groups (a scan of the certificate signed by the chairperson of the group is required).

40 points

Qualification examination

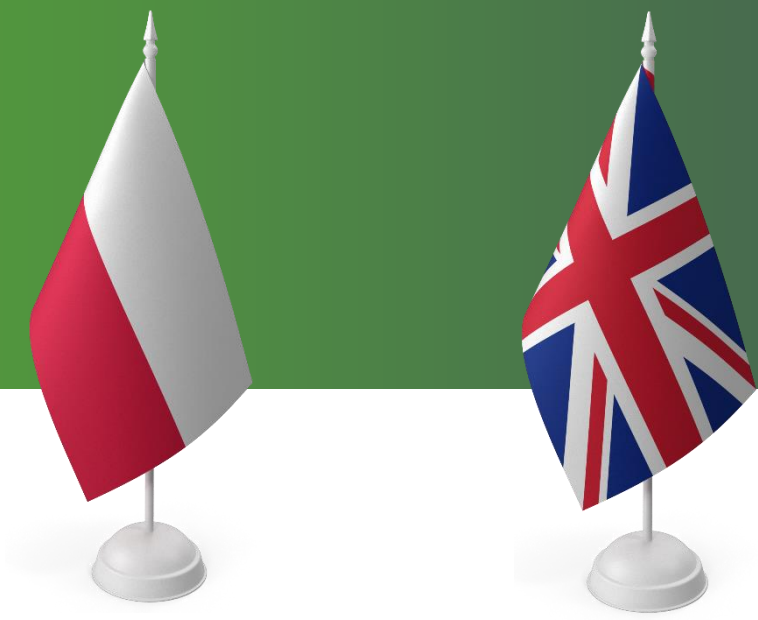
Verifying the candidate's knowledge and skills within the particular academic discipline in writing.
In justified cases (e.g. where the candidate stays abroad), at the written request of the candidate addressed to the chairperson of the qualification team appointed for the particular academic discipline, the written examination may be replaced with an oral examination carried out remotely with the use of generally available online tools.

40 points

Interview

The interview entails an assessment of the candidate's scientific potential. The interview may comprise the following elements:
1) discussion of the candidate's Master's thesis (understanding of the subject, research hypotheses, their implementation, results obtained and conclusions);
2) questions about the academic record and the course of the graduate and postgraduate studies or the uniform Master's degree studies, including subjects related to the doctoral dissertation;
3) questions pertaining to information included in letters of recommendations, including the nature and results of cooperation of the candidate with the authors of these letters;
4) questions pertaining to the doctoral project and other information included in the documentation submitted by the candidate.

The interview shall be held in Polish or English, according to candidate's preferences indicated in the IRK. If Polish is selected, a part of the interview may be held in English.



CONDITION OF ADMISSION TO THE SCHOOL

The requirement for admission to a School shall be a place on the Ranking list that is within the limit of places and getting no less than 50 points from the entire qualification procedure.

SCOPE OF THE QUALIFICATION EXAMINATION

INORGANIC AND ANALYTICAL CHEMISTRY

1. Periodic table of elements. Division into blocks s, p, d and f. Electronic configurations of elements with the following exceptions: Cr, Cu, Mo, Pd, Ag, Pt, Au. Isoelectronic atoms, ions and molecules. Covalent and ionic radius - definitions, determination and variability in the periodic table. Influence of the size and charge of ions on the acid-base properties of their connections. The concepts of: ionization energy, electron affinity, electronegativity, standard potential and their variability in the periodic table. Relationship between electronegativity and the nature of bonds. Determining the spatial shape of simple covalent molecules and molecular ions (e.g. CO_2, NH_4^+, XeF_4), taking into account the position of non-bonding electron pairs (VSEPR).

2. **Properties of selected elements and their compounds. Hydrogen.** Conditions and possibilities of H2 reaction with other elements. Metal and non-metal hydrides - classification into ionic, covalent and metallic hydrides (examples for each group). Influence of hydrogen bonds on the properties of NH_3, H_2O and HF. Application of hydrogen combustion in oxygen in a fuel cell. **Alkali and alkaline earth metals** - reactivity, reactions with water and oxygen. Water hardness and its removal. The phenomenon of amphoterism on the example of $Zn(OH)_2$ and

$Al(OH)_3$. **Carbon and silicon**. The structure of the most important allotropic forms of carbon (graphite, diamond, fullerene C60). CaC_2 carbide and its reaction with water. SiO_2 and its reaction with bases. The role of C-C and Si-O-Si bonds in the formation of carbon and silicon compounds. **Nitrogen**. Magnetic properties of the N_2 molecule. Formation of ammonia and nitric acid(V). Redox reactions of dissolution of metals in HNO_3. **Phosphorus.** Phosphorus allotropes and their structure. P_4O_{10} phosphorus oxide - structure and reactions with water. **Oxygen.** Magnetic properties of the O_2 molecule. Redox reactions involving hydrogen peroxide H_2O_2. **Sulfur.** Sulfur allotropes and their structure. The interaction of SO_2, H_2S with water. Preparation of H2SO4. **Halogens**. Physical properties and structure of elemental forms. Reactions of halogens and hydrohalides with water. **Elements of blocks d and f**. Examples of connections at different oxidation states: $Cr^{3+,}$ CrO_4^{2-}, Mn^{2+}, MnO_2, MnO_4^-, Fe^{2+}, Fe^{3+}, Prussian blue, Co^{2+}, Co^{3+}. Equations of redox reactions involving transition metal ions. Dependence of the CrO_4^{2-} / $Cr_2O_7^{2-}$ equilibrium position on the pH of the solution. Typical and unusual oxidation states of lanthanides. Influence of lanthanide contraction on basic properties of lanthanide hydroxides.

3. **Coordination compounds.** Examples of complexes with typical coordination numbers: 2 (linear), 4 (tetrahedral and planar square) and 6 (octahedral). Ethylenediamine and EDTA as multidentate (chelating) ligands. Diagram of the splitting of central-ion d orbitals in the octahedral ligand field. The concept of high and low spin complexes. The dependence of the magnetic properties of the complexes on the ligand field strength.

4. **Universal basics of chemical analysis.** Significant figures. Definition of acid and base in Brønsted's theory. Conjugate acid-base pairs. Salt hydrolysis as an acid-base reaction. Definition of acid and base in Lewis theory. pH of solutions of weak and strong acids, bases, and salts of acids and bases of different relative strength. pH of the buffer solution. The concept of the solubility product and its relationship with the molar solubility of the substance. The influence of common ion, foreign ions, protonation and complexation on the solubility of sediments.

5. **Elements of qualitative analysis.** Burner flame colors generated by volatile elements. The colors of solutions of compounds of: alkali metals, alkaline earth metals, Cr (III), Cr (VI), Mn (II), Mn (VI), Mn (VII), Fe (II), Fe (III), Co (II), Ni (II), Cu (II), Zn (II), Ag (I), Au (I), Hg (II) and Hg (I). Water solubility of chlorides, nitrates (V), sulphates (VI), sulphides and carbonates of these metals. The basis for the division of cations into analytical groups. Selected colored characteristic reactions: Fe(III) with SCN^-, Fe(III) with $Fe(CN)_6^{4-}$, Cu(II) with NH_3, Co(II) with SCN^-, Ni(II) with dimethylglyoxime. Comparison of Al(III) and Cr(III) reactions with NaOH. Distinction of Cl^-, Br^- and I^- on the basis of the reaction with $AgNO_3$.

6. **Elements of quantitative analysis. Weight analysis.** Methodology of typical determinations, e.g. sulfates in the form of $BaSO_4$ or calcium in the form of CaO. The essence of minimizing precipitate losses during washing. **Titration analysis.** Equivalence-point pH in the titrations of weak and strong acids and bases. Comparison-buffer definition. Typical pH indicators: phenolphthalein and methyl orange, and the optimal choice of indicator for a given titration. The principle of the acid-base titration of mixtures of carbonates, bicarbonates and hydroxides. Determination of calcium and magnesium with EDTA as an example of complexometric titration. **Elements of instrumental analysis.** Redox titration technique with a platinum electrode as the indicator electrode and a calomel electrode as the reference electrode. Calculation of the redox potential of a system at the equivalence point. Lambert-Beer law as the basis of absorption spectrophotometry. Molar absorption coefficient. Ilkovič equation as the basis for quantitative analysis using the polarographic method. Principle and application of the inversed voltammetric method. Potentiometry and ion selective electrodes. Atomic emission and absorption spectrometry.

ORGANIC CHEMISTRY AND BIOCHEMISTRY

1. **Hydrocarbons.** Division into classes. Hybridization of carbon atom. Structure of hydrocarbons: alkanes, cycloalkanes, alkenes, alkynes, aromatic compounds (aromatic character, Hückel's rule).

2. **Conformation:** alkanes (ethane, butane, slow rotation), cycloalkanes (ring stability). Isomerism: constitutional, geometric (cis / trans, Z / E), optical (absolute configuration R / S and its determination, Cahn-Ingold-Prelog rules; enantiomers, diastereoisomers, racemic mixture, relative configuration).

3. **Alkanes.** Synthesis and properties. Free radical substitution (SR mechanism, reaction orientation). Structure of a free radical. Stability of free radicals. Cycloalkanes: properties and reactions.
4. **Alkenes.** Synthesis and properties. Electrophilic addition of hydrogen halides and halogens (AdE mechanism, Markovnikov rule). Stability of carbocations. Free radical addition of hydrogen bromide (AdR mechanism). Hydrogenation and ozonolysis of alkenes.
5. **Alkynes.** Synthesis and properties. Alkynes (addition of hydrogen, halogen, hydrogen halide, water).
6. **Aromatic hydrocarbons (benzene).** Electrophilic substitution of aromatic compounds (SE mechanism). Nitration, sulfonation, halogenation, alkylation, acylation. Substituents effect (inductive and mesomeric effect). Alkyl derivatives of benzene, side chain substitution.
7. **Halogen derivatives.** Synthesis and properties. Haloalkanes: nucleophilic substitution, mechanisms and stereochemistry of SN1 and SN2 reactions. Elimination reactions, mechanisms E1 and E2. Reactivity of halogen derivatives: alkyl, allyl, vinyl and aromatic compounds.
8. **Alcohols.** Synthesis and properties. Classification. SN1 and SN2 substitution reactions. Elimination reactions (dehydration).
9. **Amines.** Synthesis and properties. Classification of amines. Alkylation of amines. Amine salts and quaternary ammonium salts. Aromatic amines – ring substitution. Reactions of amines with nitric (III) acid, reactions of diazonium salts.
10. **Aldehydes and ketones.** Synthesis and properties. Oxidation and reduction reactions. Nucleophilic addition (AdN) to a carbonyl group: addition of water, alcohols, hydrogen cyanide, bisulfite (bisulfate (IV)), ammonia derivatives, Grignard compounds. Cannizzaro reactions and aldol condensation (mechanisms).
11. **Carboxylic acids and their derivatives.** Synthesis and properties. Classification of carboxylic acids. Acidity of carboxylic acids - structure influence. Salts. Synthesis of acid chlorides and anhydrides, esters and amides, comparison of their reactivity. Esters: esterification and hydrolysis mechanism, Claisen condensation mechanism). Reduction of carboxylic acids and their derivatives.
12. **Heterocyclic compounds.** Heterocyclic five- and six-membered systems with one heteroatom. SE reactions of pyrrole, thiophene, furan. SE of pyridine.
13. **Multifunctional compounds.** Hydroxyketones, hydroxyaldehydes, halogen substituted carboxylic acids, amino acids, dicarbonyl compounds - synthesis and reactions. Keto-enol tautomerism.
14. **Identification of organic compounds by spectral methods.** The ability to interpret simple 1H-NMR, 13CNMR and infrared spectra (knowledge of the frequency of vibrations for basic functional groups) in order to identify compounds.
15. **Biochemistry.** Structure and function of biological membranes. Permeability and transport across membranes. The hierarchical structure of proteins (1st, 2nd, 3rd and 4th order structure). The relationship between the structure and function of proteins. Structure of enzymes, their classification, function and mechanism of action. Basic concepts of metabolism (thermodynamics of biochemical reactions, coupled reactions, compounds with high phosphorylation potential, basic principles of the organization of metabolism). Photosynthesis and biological oxidation. Structure of DNA and RNA. The flow of genetic information. Concepts of replication, transcription and translation.

PHYSICAL AND THEORETICAL CHEMISTRY

1. **Kinetic theory of gases.** Ideal and real gases. Clapeyron equation and van der Waals equation. Critical temperature. Heat capacity of ideal gases.
2. **Thermodynamics** - basic concepts. Energy, work, heat. The concept of a state function. First law of thermodynamics. Internal energy (U) and enthalpy (H), their changes in various processes.
Thermochemistry. Thermal effects of a reaction under constant pressure and constant volume. Standard enthalpy changes in physical and chemical transformations. Hess's law and its applications. Kirchhoff's law.
Entropy (S). Second law of thermodynamics. The physical significance of entropy. The dependence of S on temperature. Thermodynamically reversible and irreversible processes. Third law of thermodynamics.

Helmholtz free energy (F) and Gibbs free energy (G). Thermodynamic criteria of reaction spontaneity based on changes of S, F, and G potentials. Chemical potential. Thermodynamic equilibrium conditions.
Chemical equilibrium state. Equilibrium constant of a chemical reaction (K) and the influence of various factors (e.g., temperature) on its value. Equilibrium constant and reaction quotient expressed in partial pressures, concentrations and mole fractions. Relationship between ΔGo and K. The effect of a changes in external conditions on chemical equilibria (Le Chatelier's principle).
Phase transitions in single and multicomponent systems. Phase diagrams of pure substances (water, CO_2). Triple point. Gibbs phase rule. Raoult's law. Phase diagrams of two-component systems (positive and negative azeotropes, eutectics).
3. Electrochemistry. Electrolyte solutions. Ion solvation. Ion activity in electrolyte solutions. Activity coefficient. Debye-Hückel limiting law. The concept of an electrode and its potential. Standard potential. Nernst equation. Type I and II electrodes and typical reference electrodes: standard hydrogen, calomel, silver chloride - reactions, description of the potential by Nernst equation. pH electrodes.
Galvanic cells, types of cells and associated reactions. Theoretical calculation and experimental determination of the electromotive force (SEM). Stockholm electrochemical convention. Relation between ΔG and SEM. Determination of thermodynamic quantities from SEM measurements.
Electrolysis and transport phenomena. Faraday's law. Electrolysis of aqueous solutions of various salts - electrode reactions. Overpotential (overvoltage) of an electrode process. Diffusion and Fick's laws. Concentration gradient and diffusion coefficient. Diffusion and kinetic currents.
Colloids - electrokinetic potential. Electrophoresis and electrophoretic mobility. Isoelectric point.
4. **Chemical kinetics.** Rate of chemical reaction - definition and influence of various factors. Reaction order (partial, total), methods of determination. Kinetic equations and changes of reagent concentrations over time for reactions of various orders. The half-life of a reaction. Activation energy and Arrhenius equation. Activated complex theory. The concept and role of a catalyst.
5. **Electric and magnetic properties of substances.** Permanent and induced dipole moments of a molecule. Electric permeability and relative permittivity. Diamagnetism, paramagnetism and ferromagnetism. Magnetic susceptibility. Curie's law.
6. **Crystallography.** Basic concepts: crystal features, spherical and stereographic projection, lattice, Bravais lattices. Point symmetry, symmetry operations and symmetry elements, coexistence of symmetry elements, Schoenflies and Hermann-Maugin point group notations. Complex symmetry elements. 3D lattices, geometric objects in 3D lattices (nodes, lines and planes). Miller indices. Space groups. Close-packing and densest packing. Reciprocal lattice - definition and properties, Ewald’s sphere construction. Basics of X-ray analysis of crystals’ structure.
7. **Quantum chemistry.** Statistical interpretation of the wave function. Energy levels (degeneration, distances between the adjacent levels), wave functions (variables, the number of nodes) and quantum numbers for the following quantum systems: one-dimensional potential box (particle in a box), one-dimensional harmonic oscillator, rigid rotator, hydrogen atom and hydrogen-like ions (here also the contours of the functions s, p, d). One-electron approximation. Orbitals and spinorbitals. Wave function for a multi-electron system.
Paulie's exclusion principle. Hartree-Fock method. Electronic configurations of atoms and multi-electron ions. Hund's rule. Atomic term symbols (the base term of a multi-electron atom). Born-Oppenheimer approximation. Molecular orbitals (MO) method. LCAO MO method. Mechanism of chemical bond formation in terms of the MO method. Molecular orbitals in diatomic homonuclear molecules (σg, σu, πg, πu). Bonding, anti-bonding and non-bonding orbitals. Energy levels and electronic configurations in homonuclear diatomic molecules of elements from the second period and simple heteronuclear diatomic molecules. Potential energy diagrams for a diatomic molecule (vibrational and rotational levels). Molecular orbitals method for polyatomic molecules. Orbital hybridization. Hybridized orbitals of the following types: sp, sp^2, sp^3.
8. **Spectroscopy.** The nature and properties of electromagnetic radiation. Energy quantization of rotational, vibrational (including anharmonic vibrations), and electronic states in a molecule. Boltzmann distribution and relative population of energy levels. Electromagnetic radiation frequency (and wavelength) range and the observed types of spectral transitions. Selection

rules in rotational and vibrational absorption spectroscopy. Inelastic scattering: Stokes and anti-Stokes bands. Selection rules in vibrational Raman spectroscopy. Relative position of absorption and emission peaks in luminescence spectroscopy (fluorescence and phosphorescence). EPR spectroscopy. Hyperfine structure of EPR spectra. NMR spectroscopy: interaction of atomic nuclei of non-zero magnetic moment with an external magnetic field, nuclear shielding and chemical shifts. Interactions of magnetic nuclei (spin-spin coupling).

CHEMICAL TECHNOLOGY AND FUNDAMENTALS OF BIOTECHNOLOGY

1. **Fundamentals of chemical technology.** Unit operations and processes. Effectivity, yield, selectivity and Energy consumption as essential parameters of technological process evaluation. Material and Energy balances. Chemical and physical laws employed in material and energy balances preparation. The features of novel and green technologies. Waste Management in Chemical Technologies - environmental protection aspect.
2. **Technology rules:** sustainable utilization of sources, energy, instrumentation. Economic optimization of technological process. Designing of the technological process on a larger scale.

CONTACT

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