The ministry of science and higher education of the Russian Federation
Federal state autonomous educational institution of higher education «Ural federal university named after the first President of Russia B. N. Yeltsin»
Institute of chemical engineering

APPROVED
Vice-rector for Research
A. V. Germanenko

DISCIPLINE WORKING PROGRAM
Technology of organic substances

List of information about the discipline working program	Credentials
Doctoral program Technology of organic substances	**Code DP** 2.6.10
Group of specializations Chemical technologies, material sciences, metallurgy	**Code** 2.6.
Federal state requirements (FSR)	Order of the Ministry of science and higher education of the Russian Federation of 20.10.2022 № 951
Independently approved requirements (IAR)	Order «On the introduction of «Requirements to the development and implementation of academic staff training programs in the UrFU doctoral course» of 31.03.2022 № 315/03

Yekaterinburg

2023

Discipline working program is compiled by:

№	Full name	Academic degree, academic title	Occupational title	Research unit
1	Zyrianov Grigory Vasil'evich	D.Sc., Professor	Professor	Department of organic and biomolecular chemistry
2	Glukhareva Tatiana Vladimirovna	PhD, Associate Professor	Associate Professor	Department of technology for organic synthesis

Recommended by educational and methodological board of the Institute of chemical engineering:

Chairman of the educational and methodological board of the institute A. B. Darintseva

Report № 1 of 10.01.2023

Agreed by:

Head of academic staff training department E. A. Butrina

1. GENERAL DESCRIPTION OF THE DISCIPLINE «TECHNOLOGY OF ORGANIC SUBSTANCES»

1.1. Annotation of the discipline content

The discipline **«TECHNOLOGY OF ORGANIC SUBSTANCES»** refers to the basic part of the doctoral program and is aimed at training of highly qualified competent specialists in the field of organic chemistry.

The aim of the discipline: obtaining knowledge by doctoral students on the technology of organic substances.

The study of the discipline involves the following tasks:

- the study of the theoretical foundations of organic chemistry and the mechanisms of organic reactions;
- the study of methods for the synthesis of organic compounds and prospects for the development of the organic synthesis industry;
- the study of the principles of organic synthesis technology, chemical reactors for the organic synthesis processes;
- the study of the physical and chemical foundations of organic synthesis processes;
- acquisition of new scientific knowledge in the field of theoretical foundations and practices of using separation and reaction-mass transfer processes in the organic synthesis industry;
- skills formation for the development of optimal technological schemes for the production of organic compounds, computerized design, production design, and management.

1.2. The language of the discipline implementation - Russian.

1.3. Expected discipline learning outcomes

As a result of mastering the discipline, the doctoral student should:

Know:

- structure and basic properties of organic substances;
- research methods of organic substances;
- physical and chemical foundations of technology of organic substances;
- the main regularities of the processes of technology of organic substances;
- technologies for the production of basic products of organic synthesis.

Be able to:

- use research methods for organic substances;
- use physics and chemistry and the main regularities of processes for the development of technologies for organic substances;
- develop energy-, resource-saving, and environmentally friendly technologies for the synthesis of organic substances.

Demonstrate:

- modern research methods of organic substances;
- energy-, resource-saving, and environmentally friendly technologies for the synthesis of organic substances;
- manage the formation processes of the structure and specified properties of organic substances;
- skills of working with the scientific literature to determine the research direction and solve specialized problems.

1.4. Discipline loads

#	Types of the educational work	Discipline load		Discipline load distribution in the 6th semester (hours)
		Total hours	Including work with a lecturer (hours)*	
1.	Classwork	4		4
2.	Lectures	4	4	4
3.	Independent work of doctoral students, including all types of continuous assessments	104	1	104
4.	Midterm assessment	104	1	E
5.	Total load of curriculum, hours	108		108
6.	Total load of curriculum, credit points	3		3

*Work with a lecturer includes:
in #2, 3 – the number of hours equal to the corresponding type of work;
in #4 – the number of hours equal to the time devoted by a lecturer to the meeting with the group (15% of the load of classwork);
in #5 –the number of hours equal to the time devoted by a lecturer to perform the corresponding type of midterm assessment of a doctoral student.

2. DISCIPLINE CONTENT

#	Section, discipline topic	Content
S1	Theoretical foundations of organic chemistry and reaction mechanisms of organic compounds	Definition of the concept of «reaction mechanism». Factors determining the implementation of an elementary step between reacting species: electronic (the formation of reaction centers) and steric (accessibility of reaction centers). Quantum-chemical calculations of reactivity. Analysis of the reactivity of organic compounds using MO theory. Classification of reagents. Nucleophilic, electrophilic, and radical reagents. Their features and main types. Classification of reactions. Classification by chemical nature (substitution, addition, elimination reactions, molecular rearrangements) and by the nature of the change in bonds. Substitution reactions. General characteristics. Features of aromatic compounds. Hückel's rule. Aromatic carbocations and carbanions. Heterocyclic compounds. Electrophilic substitution; π- and σ-complexes. Mechanism and kinetics of electrophilic substitution reactions. Orientation in electrophilic substitution. Influence of substituents on the electron density distribution in the ground and transition states. The relative rate constant. The steric effect of substituents.

		Nucleophilic substitution. Features of nucleophilic substitution at unsaturated and saturated carbon atoms. Features of nucleophilic substitution reactions in aromatic compounds. The reaction mechanism - monomolecular, bimolecular (addition-elimination), benzyne, ion-radical. Radical substitution. Reaction mechanism. Influence of various factors. The ratio of isomers. Formation and stability of radicals. Radical reactions proceeding by chain mechanisms. Addition reactions. General characteristics. Reactions of nucleophilic, electrophilic, and radical addition. Markovnikov's rule and the Karash effect. Elimination reactions. General characteristics. Bimolecular and monomolecular elimination.
S2	Methods for synthesis of organic compounds	Halogenation. Direct halogenation, basic methods, and their comparative evaluation. The use of hydrogen halides, the mechanism, and the regiospecificity of the reaction. The use of sulfur and organophosphorus halides. Substitution of a halogen atom with other atoms and groups. Substitution with a hydroxyl group, a cyano group, etc. Sulfonation. The introduction of a sulfo group into aliphatic and aromatic compounds. Sulfochlorination. Sulfamides, their synthesis, and properties. Sulfanilamide drugs. Substitution of the sulfo group with other atoms and groups. Nitration. Introduction of a nitro group into aliphatic and aromatic compounds. Reagents, reaction conditions. Transformations of the nitro group. Examples of the use of the nitration reaction in the synthesis of biologically active compounds. Nitrosation. Reagents and reaction conditions. The use of the nitrosation reaction, the synthesis of Pyramidon and Analgin. Nitrosation at the nitrogen atom. Diazomethane and diazoalkanes. Diazotization. Reaction mechanism and conditions. Properties of diazo compounds, their analysis. Azo coupling reactions. Use of azo coupling reactions. Diazo transformations. Synthesis of pyrazolones. Deamination, Griess method, and new modifications. Sandmeyer reaction. Substitution of the diazo group with other substituents. Oxidation. General trends. Oxidation reactions at the carbon atom. Oxidation of methyl and methylene groups of primary and secondary alcohols, aldehydes, and ketones, carboxylic acids. The most common reagents, reaction conditions. Oxidation reactions and catalytic dehydrogenation. Oxidation of multiple carbon-carbon bonds. Reagents for the oxidation of double and triple bonds, glycol cleavage. Oxidative cleavage of secondary alcohols and ketones. Reduction. Types of reduction reactions. Hydrogenation. Catalysts, theory of catalysis, classification of catalysts. Homogeneous and heterogeneous catalysis. Reduction reactions resulting from the transfer of the hydride ion. Nucleophilic hydrides. Complex hydrides. Reduction examples. Reduction with organometallic compounds. Grignard reagents. Reduction under the action of metals (Na, Mg, Zn). Reaction conditions, mechanism, stereochemistry. Redox reactions. Oppenauer-Meerwein-Ponndorf reactions. Conditions and mechanism. Cannizzaro-Tishchenko reaction.

		Reactions of organoelement compounds (OEC). OEC classification. Methods of synthesis and properties. Features of organometallic compounds of magnesium, zinc, cadmium, aluminum, and lithium. The use of OEC in fine organic synthesis. Methods for the synthesis of organomercury, organoarsenic, and organophosphorus compounds. Their application in the chemistry of biologically active compounds. Boron compounds. Preparation methods and reactions. Acylation. Friedel-Crafts reaction, conditions. Examples of use in the chemistry of biologically active compounds. Formylation of aromatic compounds. Vilsmeier reaction. Conditions, reagents. Phosphorylation. Phosphorylation reactions for the synthesis of phosphoric acid mono-, di- and triesters. The mechanism of formation. Possible side reactions. Synthesis strategy. Phosphoric acid activation methods. Chlorophosphate method, use of mixed phosphoric anhydrides, dicyclohexylcarbodiimide method, reactions with phosphatins. Advantages and limitations of methods. Use of protecting groups in fine organic synthesis and chemistry of biologically active compounds. Protection of C-N-bonds in acetylenic and aromatic compounds. Protection of NH bonds. Formation of a new N-C bond. Synthesis of urethane derivatives. Alkyl and aryl derivatives. Silyl protection. Protection of the hydroxyl group. Protections of the carboxylic groups. Methods for the synthesis of various esters, their stability, and deprotection methods. Protection of thiols by introducing protecting groups through modification of the sulfhydryl substituent. Protection methods for aldehydes and ketones. Protection of multiple carbon-carbon bonds. Condensation reactions. Types of reactions. The reaction of carbonyl compounds with C-H acids. Strecker amino acid synthesis. Aldon condensation. Reaction conditions. Knoevenagel reaction, Perkin reaction, etc. Darzens glycidic ester condensation. Claisen condensation. Michael reaction and its use in natural product synthesis. Mannich reaction. Wittig reaction, reagents, reaction conditions, regio- and stereospecificity. Diels-Alder reaction. Dakin-West, Arndt-Eistert reactions. Knorr reaction. Bischler-Napieralski reaction. Rearrangements. Classification of rearrangement reactions, occurring through the formation of a charge that is not conjugated with multiple bonds. Migration of a carbon substituent from one carbon atom to another carbon atom. Nucleophilic and electrophilic rearrangements. The formation of a positive charge on the carbon atom due to the polarization of the double bond, the elimination of the halogen, hydroxyl, and diazo groups. The positive charge on the nitrogen atom, methods of formation. Rearrangements triggered by the formation of a charge on oxygen. Allylic rearrangements. Radical, nucleophilic, and electrophilic rearrangements. Transfer of a substituent from carbon to carbon, from heteroatom to carbon. Use of new reagents in fine organic synthesis. Polymer-supported reagents, their application, and their advantages. Phase-transfer catalysis with heterogeneous reagents. Crown ethers. Examples of the use of new reagents in the chemistry of natural products.
S3	Principles of organic synthesis technology	The main trends in the development of organic synthesis (OS) as an industry. The specifics and system regularities of this industry. Ecological characteristics of the industry and its individual producing units. Problems

		facing the organic synthesis industry. General approaches to the creation of waste-free energy-saving industries and their development prospects. Key principles used in the creation of non-waste industries and their classification. Methodological principles. The role of a systematic approach in the creation of non-waste industries. Chemical principles. Creation of few-step chemical productions. Development of methods for the production of products from affordable and cheap raw materials. Development of highly effective processes. The use of «coupled» methods for obtaining products. Development of technologies that allow high conversions. Combination of several reactions aimed at obtaining the same target product. Technological principles. The use of component and flow recirculation. The use of combined processes. The separation efficiency of the products from the reaction mixture. Development of processes with low energy consumption. The efficiency of the use of the system energy. Development of technology with minimal water consumption and the use of its circulation. The efficiency of the gas flow usage and purification of gas emissions. The use of large unit capacity apparatus and technological lines. Application of continuous processes. Completeness of liquid and solid waste utilization. High level of automation. High reliability and stability assurance of the chemical-engineering system. Organizational principles and features of their application to the creation of non-waste production. The need to use the full set of principles (i.e. a systematic approach) to assess the technology effectiveness. The concept of extremely efficient technology. Economic feasibility of non-waste technology. Approach to the development of non-waste production. The sequence of choice of optimum alternative for non-waste technology.
S4	Physics and chemistry of organic synthesis processes	Fundamentals of thermodynamics of chemical processes and phase equilibrium. Thermodynamic regularities of chemical and phase equilibria for real multicomponent systems. Characteristic functions, chemical potentials. Concept of activity and activity coefficients, methods for their calculation, and experimental determination for real gases and liquids (solutions). Principles of phase and chemical equilibria calculation for real multicomponent systems and complex reactions. Law of mass action. Stoichiometric analysis of complex reactions. The extent of reaction. Thermodynamic analysis of the most important reactions of organic synthesis (chlorination, oxidation, hydrogenation and dehydrogenation, hydration and dehydration, esterification and hydrolysis, carbonylation and alkylation, etc.) and the choice of their reaction conditions. Mathematical modeling of liquid-vapor, liquid-liquid, liquid-liquid-vapor, and liquid-solid phase equilibria. Azeotrope, chemiazeotrope and polyazeotrope. Phase equilibrium laws (Raoult's law and Dalton's law). Statics analysis of multiphase reaction systems with selective exchange with the environment. Basic concepts thermodynamic topological analysis, the structure of equilibrium phase diagrams. Kinetics, mechanism, and catalysis of organic reactions. Active species (intermediates) in organic synthesis. Ions, radicals, carbenes, radical ions, metal complexes, and organometallic compounds. Fundamentals of reactivity theory for organic compounds. Relationship between kinetics and

		thermodynamics. Bell–Evans–Polanyi principle. Bronsted, Hammett, Taft, Polanyi-Semenov equations. Selection rules for elementary steps in the reaction mechanism hypothesizing. Heterolytic and homolytic mechanisms. Nucleophilic and electrophilic substitution, addition, and elimination reactions in organic synthesis. Kinetics and mechanism of these reactions. The influence of the reaction medium. Acid and basic catalysis in heterolytic reactions. Protic and aprotic acids. Industrial catalysts. Mechanism of reactions and features of kinetics of hydration, dehydration, alkylation, polymerization, hydrolysis, esterification, and cracking processes. Radical chain processes in industrial organic synthesis. Mechanism, initiators, catalysts, inhibitors. Kinetic models of chlorination, oxidation, pyrolysis, and polymerization reactions. Metal complex catalysis in industrial organic synthesis. The structure of metal complexes. Nature and mechanism of the main steps of metal complex-mediated reactions. Features of the kinetics of metal complex-mediated reactions. Catalysts and mechanism of the methanol carbonylation, hydroformylation, olefin oxidation with oxygen and hydroperoxides, hydrogenation and polymerization processes, olefin metathesis. Heterogeneous catalysis in industrial organic synthesis. Catalysis with metals, oxides, and polyfunctional catalysts. The mechanism of hydrogenation, oxidation, oxidative ammonolysis, and syntheses from CO and H_2. Influence of mass transfer processes on the kinetics of heterogeneous catalytic reactions. Kinetics under conditions of kinetic, external, and internal diffusion regions. heterophase processes. Peculiarities of kinetics in the case of slow and instantaneous chemical reactions, taking into account the influence of diffusion. Theoretical foundations for kinetic modeling of complex multi-route organic reactions. Route theory. Methods for kinetic data analysis and mathematical description of the product composition and selectivity for complex reactions: sequential, parallel, sequential parallel.
S5	Chemical reactors for organic synthesis processes	Ideal reactors. Main types of real reactors. Experimental determination of the flow structure and a set of chemical reactors. Classification of chemical reactors. Features of the use of chemical process kinetic models in the mathematical modeling of the reactor. Principles for calculating reactor sizing, product composition, and selectivity from kinetic data with account for the reactor model and heat balance equations. Choice of reactor types based on their productivity, reaction selectivity, and thermal and kinetic characteristics of the process. Optimization principles of process parameters based on thermodynamic and kinetic data, the use of economic criteria for optimality. Characteristics of constructions, material flows, thermal condition, and choice of technological design of the reaction unit for the main homogeneous, heterogeneous catalytic, and heterophase processes of industrial organic synthesis. Application of fluidized bed reactors, sectioning equipment, and flow optimization in reactors. Reaction heat and hot flows utilization, energy, and exergy efficiency of reactors. Reactors with a combination of chemical and separation processes.

S6	Theoretical foundations and practice of separation and reaction-mass transfer processes in organic synthesis industry	Scientific foundations of standard cleaning methods of raw materials from harmful impurities and their drying. Features of raw materials treatment scheme for chlorination, oxidation, hydrogenation, and other processes. Scientific foundations for the separation of real multicomponent mixtures by rectification, extraction, extractive and azeotropic rectification, liquid extraction, absorption, adsorption, chemisorption, etc. The principle of concentration field redistribution between separation areas. Choice of extractants, extractive and azeotropic agents, sorbents: characteristics of their separating ability. Fundamentals of separation processes statics. Synthesis and analysis of technological separation schemes. Separation of polyazeotropic multicomponent homogeneous and exfoliating mixtures. Kinetics of heat and mass transfer, separation equipment modeling, calculation methods. Comparative evaluation and selection of separation methods for multicomponent mixtures, technological separation schemes, and the corresponding equipment. Optimization of separation processes and technological schemes. The concept of a separation complex of a functional action. Typical complexes and schemes for processing and separation of basic organic chemicals. Comparison of combined and recirculation design options for reaction-mass transfer processes. The general strategy for research and development of reaction mass-transfer processes. Evaluation of the separation effect on the conversion level and selectivity of the reaction. Application of statics analysis to identify the optimal options for organizing reaction-rectification processes. Methods of purification of sewage, and waste gases in the industry of organic synthesis.
S7	The use of computers in the creation, design, and production management	Mathematical description of chemical transformation processes, kinetic models. Mathematical models of chemical reactors. Calculation of their parameters using a computer. Mathematical modeling of liquid-vapor, liquid-liquid, and liquid-liquid-vapor phase equilibria, including those with a chemical reaction. Computer modeling of mass transfer equipment, and manufacturing facilities. Modeling fundamentals of combined reaction-rectification processes and equipment for their implementation. The role of computers in the automation of research, technological equipment design, and management.
S8	Prospects for the development of the organic synthesis industry	Basic concepts for the development of the organic industry synthesis. Ways of saving in material, energy, and human resources consumption, cost savings. Solving environmental and safety problems. Ways of combining to solve these problems. A common use of zero-waste principles in the development of industrial processes of organic synthesis. The combination of various reactions with mass transfer processes, the combination of several reactions, and several mass transfer processes aiming to carry them out in one apparatus. Physics and chemistry and technological principles of creation of directly-combined reaction-rectification processes. Ways to organize and optimize them. Issues of system approach in the development, design, and analysis of basic organic chemical manufacturing. Historical development, current state, and expansion prospects of organic synthesis raw material base. Ways to improve the production of olefins, aromatic hydrocarbons, acetylene, carbon monoxide, etc.

/		Historical development, current state, prospects, and ways to improve the basic processes of organic synthesis based on the study of system-wide regularities and methods to improve their economic efficiency. Improvement of the reliability, and resilience of technological units and individual instruments, measures to reduce technological units by combining processes and stages, the introduction of equipment, technological lines of large unit capacity, and the development of the foundations of material and energy-saving technologies. Development and application of automated systems for scientific research and production design.

3. ORGANIZATION OF PRACTICE AND INDEPENDENT WORK IN THE DISCIPLINE

3.1. Practice

Not provided.

3.2. Approximate topic of independent work

3.2.1. Approximate list of essay topics

The topics of essays should consider an analytical review of scientific, technical, and patent literature on the problem solved by a doctoral graduate student while working on a thesis.

1. Physical chemistry of synthesis, production engineering, composition, properties, and application of heterocyclic compounds.
2. Physical chemistry of synthesis, production engineering, composition, properties, and application of biologically active compounds.
3. Physical chemistry of synthesis, production engineering, composition, properties, and application of photoactive compounds.

The essay volume is 20-25 typewritten pages in A-4 format.

3.2.2. Approximate topics of individual or group projects

Not provided.

4. THE SET OF TOOLS FOR CONTINUOUS AND MIDTERM DISCIPLINE ASSESSMENT

4.1.The evaluation criteria for the results of the control test activities of continuous and midterm doctoral research assessment

Approved evaluation criteria of the achievements of doctoral students for each control test activity are applied. The evaluation criteria system is based on three levels of mastering the competence components: intermediate, advanced, and high.

Competence components	Indications of the level of competence components acquisition		
	intermediate	**advanced**	**high**
Knowledge	The doctoral student demonstrates knowledge-familiarity, and knowledge-copy: recognizes objects, phenomena, and concepts, finds differences between them, shows knowledge of the information sources, and can independently perform reproductive actions on knowledge by independently reproducing and applying information.	The doctoral student demonstrates analytical knowledge: confidently reproduces and understands the acquired knowledge, assigns it to one or another classification group, independently systematizes it, establishes relationships between them, and applies it productively in familiar situations.	The doctoral student is able to independently extract new knowledge from the world, and creatively apply it for problem-solving in new and non-standard situations.
Skills	The doctoral student is able to correctly follow the prescribed instructions and algorithms in a familiar situation, and independently solves typical tasks that require choosing from known methods in a predictably changing situation.	The doctoral student is able to independently perform actions techniques, and operations) to solve non-standard tasks that require a choice based on a combination of known methods in an unpredictably changing situation.	The doctoral student is able to independently solve research problems and demonstrates the creative application of skills (technologies).
Personality	The doctoral student has low motivation for learning, and shows an indifferent, irresponsible attitude to learning and assigned work.	The doctoral student demonstrates high motivation to learning, shows a positive attitude towards study and the future career, and demonstrates activity.	The doctoral student demonstrates strong motivation to learning and work, and shows persistency, enthusiasm, diligence, independence, and creativity.

4.2. The tools for continuous and midterm assessments

The list of sample review questions to prepare for the assessment (tested competencies GTC-1, GTC-2, GTC-3, GTC-6, TC-1, TC-2, TC-3, TC-4, TC-5):

1. Classification of reagents. Nucleophilic, electrophilic, and radical reagents. Their features and main types.
2. Classification of reactions. Classification by chemical nature (substitution, addition, elimination reactions, molecular rearrangements) and by the nature of the change in bonds.
3. Substitution reactions. General characteristics. Features of aromatic compounds. Hückel's rule. Aromatic carbocations and carbanions. Heterocyclic compounds.
4. Electrophilic substitution; π- and σ-complexes. Mechanism and kinetics of electrophilic substitution reactions.
5. Orientation in electrophilic substitution. Influence of substituents on the electron density distribution in the ground and transition states. The relative rate constant. The steric effect of substituents.
6. Nucleophilic substitution. Features of nucleophilic substitution at unsaturated and saturated carbon atoms. Features of nucleophilic substitution reactions in aromatic compounds. The reaction mechanism -monomolecular, bimolecular (addition-elimination), benzyne, ion-radical.
7. Radical substitution. Reaction mechanism. Influence of various factors. The ratio of isomers. Formation and stability of radicals. Radical reactions proceeding by chain mechanisms.
8. Addition reactions. General characteristics. Reactions of nucleophilic, electrophilic, and radical addition. Markovnikov's rule and the Karash effect.
9. Elimination reactions. General characteristics. Bimolecular and monomolecular elimination.
10. Halogenation. Direct halogenation, basic methods, and their comparative evaluation. The use of hydrogen halides, the mechanism, and the regiospecificity of the reaction.
11. The use of sulfur and organophosphorus halides. Substitution of a halogen atom with other atoms and groups. Substitution with a hydroxyl group, a cyano group, etc.
12. Sulfonation. The introduction of a sulfo group into aliphatic and aromatic compounds. Sulfochlorination. Sulfamides, their synthesis, and their properties. Sulfanilamide drugs. Substitution of the sulfo group with other atoms and groups.
13. Nitration. Introduction of a nitro group into aliphatic and aromatic compounds. Reagents, reaction conditions. Transformations of the nitro group. Examples of the use of the nitration reaction in the synthesis of biologically active compounds.
14. Diazotization. Reaction mechanism and conditions. Properties of diazo compounds, their analysis. Azo coupling reactions. Use of azo coupling reactions. Diazo transformations.
15. Oxidation. General trends. Oxidation reactions at the carbon atom. Oxidation of methyl and methylene groups of primary and secondary alcohols, aldehydes, and ketones, carboxylic acids. The most common reagents, reaction conditions.
16. Reduction. Types of reduction reactions. Hydrogenation. Catalysts, theory of catalysis, classification of catalysts. Hydrogenolysis. New bonds formation through hydrogenation.
17. Use of protecting groups in fine organic synthesis and chemistry of biologically active compounds.
18. The main trends in the development of organic synthesis (OS) as an industry. The specifics and system regularities of this industry. Ecological characteristics of the industry and its individual producing units.

Methodological principles. The role of a system approach in the creation of non-waste industries.

19. Chemical principles. Creation of few-step chemical productions. Development of methods for the synthesis of products from affordable and cheap raw materials. Development of highly effective processes.

20. Radical chain processes in industrial organic synthesis. Mechanism, initiators, catalysts, inhibitors. Kinetic models of chlorination, oxidation, pyrolysis, and polymerization reactions.
21. Metal complex catalysis in industrial organic synthesis. The structure of metal complexes. Nature and mechanism of the main steps of metal complex-mediated reactions.
22. Chemical reactors for organic synthesis processes. Ideal reactors. Main types of real reactors. Experimental determination of the flow structure and a set of chemical reactors. Classification of chemical reactors.

4.2.1. List of sample questions for test

Not provided.

4.2.2. List of sample questions for the exam

1. Definition of the concept of «reaction mechanism». Factors determining the implementation of an elementary step between reacting species: electronic (the formation of reaction centers) and steric (accessibility of reaction centers).
2. Electrophilic substitution; π- and σ-complexes. Mechanism and kinetics of electrophilic substitution reactions.
3. Classification of reagents. Nucleophilic, electrophilic, and radical reagents. Their features and main types.
4. Classification of reactions. Classification by chemical nature (substitution, addition, elimination reactions, molecular rearrangements) and by the nature of the change in bonds.
5. Addition and elimination reactions. General characteristics. Nucleophilic, electrophilic, and radical addition reactions. Elimination reactions. General characteristics. Bimolecular and monomolecular elimination substitution.
6. Oxidation reactions and catalytic dehydrogenation. Oxidation of multiple carbon-carbon bonds. Reagents for the oxidation of double and triple bonds. Glycol cleavage. Oxidative cleavage of secondary alcohols and ketones.
7. Heterolytic and homolytic mechanisms. Nucleophilic and electrophilic substitution, addition, and elimination reactions in organic synthesis. Kinetics and mechanism of these reactions. The influence of the reaction medium. Acid and basic catalysis in heterolytic reactions.
8. Acylation. Friedel-Crafts reaction, conditions. Examples of use in the chemistry of biologically active compounds. Formylation of aromatic compounds.
9. Carboxylic acids and their derivatives. Methods of acid synthesis: oxidation of primary alcohols and aldehydes, alkenes, alkynes, alkylbenzenes, hydrolysis of nitriles and other carboxylic acids derivatives, synthesis based on organometallic compounds, syntheses based on the malonic ester.
10. Reactions of carboxylic acids: Hell–Volhard–Zelinsky halogenation, ketonization, Kolbe electrolysis, Hunsdiecker decarboxylation. Methods for the synthesis of carboxylic acids derivatives: halides, anhydrides, esters, nitriles, amides. Ketenes, their preparation, and properties.
11. Introduction of a nitro group into aliphatic and aromatic compounds. Reagents, reaction conditions. Transformations of the nitro group. Examples of the use of the nitration reaction in the synthesis of biologically active compounds. Nitration. Nitrating agents. Mechanism of nitration reactions. Nitration of benzene and its derivatives.
12. Methods for the synthesis of aldehydes and ketones: from alcohols, carboxylic acids derivatives, alkenes (ozonolysis), alkynes (hydroboration), and organometallic compounds. Acylation and formylation of arenes.

13. Nucleophilic substitution. Features of nucleophilic substitution at unsaturated and saturated carbon atoms.
14. Features of nucleophilic substitution reactions in aromatic compounds. The reaction mechanism - monomolecular, bimolecular (addition-elimination), benzyne, ion-radical.
15. The introduction of a sulfo group into aliphatic and aromatic compounds. Sulfochlorination. Sulfamides, their synthesis, and properties. Sulfanilamide drugs. Substitution of the sulfo group with other atoms and groups.
16. Friedel-Crafts reaction, conditions. Examples of use in the chemistry of biologically active compounds. Formylation of aromatic compounds. Vilsmeier reaction. Conditions, reagents.
17. Methods for the synthesis of amines: Hoffmann alkylation of ammonia and amines, Gabriel alkylation of potassium phthalimide, reduction of nitrogen-containing derivatives of carbonyl compounds and carboxylic acids, nitro compounds, alkyl azides. Hoffmann rearrangement and Curtius rearrangement. Synthesis of amines with a tertiary alkyl radical (Ritter reaction), the reaction of aldehydes and ketones with ammonium formate (Leuckart reaction). Reactions of amines. Alkylation and acylation.
18. Nitrosation and diazotization reactions. Reagents and reaction conditions. The use of the nitrosation reaction, the synthesis of Pyramidon and Analgin. Nitrosation at the nitrogen atom. Diazomethane and diazoalkanes. Azo coupling reactions. Use of azo coupling reactions. Diazo transformations. Sandmeyer reaction. Substitution of the diazo group with other substituents.
19. Rearrangements. Classification of rearrangement reactions. Reactions occurring through the formation of a charge that is not conjugated with multiple bonds. Migration of a carbon substituent from one carbon atom to another carbon atom. Nucleophilic and electrophilic rearrangements.
20. Reactions of organoelement compounds (OEC). OEC classification. Methods of synthesis and properties. Features of organometallic compounds of magnesium, zinc, cadmium, aluminum, and lithium.
21. Catalysts, theory of catalysis, classification of catalysts. Homogeneous and heterogeneous catalysis.
22. Use of protecting groups in fine organic synthesis and chemistry of biologically active compounds. Protection of C-N-bonds in acetylenic and aromatic compounds. Protection of NH bonds. Formation of a new N-C bond. Synthesis of urethane derivatives. Alkyl and aryl derivatives. Silyl protection. Protection of the hydroxyl group. Protections for carboxylic groups.
23. Use of new reagents in fine organic synthesis. Polymer-supported reagents, their application, and their advantages. Phase-transfer catalysis with heterogeneous reagents. Crown ethers. Examples of the use of new reagents in the chemistry of natural products.
24. Mass spectrometry. Methods of ionization and separation of ions by mass. Spectrum characteristics. Use for the structure determination of organic compounds.
25. ^{1}H NMR spectroscopy. Principle of the method and characteristics of the spectrum.
26. ^{19}F, ^{31}P, ^{14}N, ^{15}N, ^{11}B NMR spectroscopies. Principle of the methods and characteristics of the spectra in comparison with ^{1}H NMR spectroscopy.
27. ^{13}C NMR spectroscopy. Principle of the method and characteristics of the spectrum compared with ^{1}H NMR spectroscopy.
28. IR spectroscopy. Use in organic synthesis.
29. Electronic spectroscopy. Use in organic synthesis.
30. Scientific foundations of standard purification methods of raw materials from harmful impurities and their drying. Features of raw materials treatment scheme for chlorination, oxidation, hydrogenation, and other processes.

31. The main trends in the development of organic synthesis (OS) as an industry. The specifics and system regularities of this industry. Ecological characteristics of the industry and its individual producing units.
32. Issues of system approach in the development, design, and analysis of basic organic chemical manufacturing. Historical development, current state, and expansion prospects of organic synthesis raw material base. Ways to improve the production of olefins, aromatic hydrocarbons, acetylene, carbon monóxide, etc.
33. Historical development, current state, prospects. The main trends in the development of organic synthesis (OS) as an industry. The specifics and system regularities of this industry. Ecological characteristics of the industry and its individual producing units.
34. Methods of purification of sewage, and waste gases in the industry of organic synthesis.
35. Comparative evaluation and selection of separation methods for multicomponent mixtures, technological separation schemes, and the corresponding equipment. Optimization of separation processes and technological schemes. The concept of a separation complex of a functional action. Typical complexes and schemes for processing and separation of basic organic chemicals.
36. Comparison of combined and recirculation design options for reaction-mass transfer processes. The general strategy for research and development of reaction mass-transfer processes.
37. Chemical reactors for organic synthesis processes. Mathematical description of chemical transformation processes, kinetic models. Mathematical models of chemical reactors. Calculation of their parameters using a computer.

5. EDUCATIONAL, METHODOLOGICAL, AND INFORMATIONAL SUPPORT

5.1. Recommended literature

5.1.1. Main literature

1. Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry. Part A: Structure and Mechanisms.* Springer: New York, 2008; p 1199.

2. Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry. Part B: Reaction and Synthesis.* Springer: New York, 2007; p 1321.

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5.2. Institute teaching and learning materials

Not provided

5.3. Software

1. Microsoft office (Word, Excel, Power point)
2. Adobe Reader
3. ChemOffice (ChemDraw Professional)
4. ISIS/Draw

5. CorelDraw X5
6. Mercury
7. Olex2
8. OriginLab
9. Mathcad 2014

5.4. Databases, information reference, and search systems

1. ScienceDirect https://www.sciencedirect.com/
2. Web of Science https://www.webofknowledge.com
3. Scopus: http://www.scopus.com
4. SciFinder: http://www.scifinder.com
5. Reaxys: http://reaxys.org
6. Academic Search Ultimate EBSCO publishing http://search.ebscohost.com
7. Federal Institute of Industrial Property https://www1.fips.ru/en/
8. Search system Google Search https://www.google.com/

5.5. Electronic learning sources

1. Zonal scientific library http://lib.urfu.ru/course/view.php?id=167
2. UrFU electronic resources http://lib.urfu.ru/mod/data/view.php?id=2802
3. Library catalogue http://lib.urfu.ru/course/view.php?id=181

6. LOGISTIC DISCIPLINE SUPPORT

6.1. Details on the specialized and laboratory equipment availability

Ural Federal University has specialized premises for lectures, group and individual meetings, continuous and midterm assessments, premises for independent student work as well as premises for equipment storage and preventive maintenance.