

ABSTRACT

of the dissertation for the PhD degree
in specialty 6D072000 – Chemical technology of inorganic substances

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“Determination of regularities of changing in the chemical and phase composition, structure and physicochemical properties of water-salt systems, their applied significance for halurgic technology»

Relevance of the dissertation. Water-salt systems are often used in the technology of inorganic substances including halurgic technologies; they are a unique basic interaction center. Studying the regularities of compositional, phase, structural, and physicochemical changes in these systems is of great scientific and applied importance. Since the halurgic technologies, applied for separation of mineral raw materials from aqueous solutions in the form of mixtures of various salts and also pure, impurity-free individual salts, fully depends on these regularities, their target achievements are the results of compositional, phase, structural and physicochemical changes in water-salt systems. The main elementary material particles in water-salt systems are atoms and ions. Their sizes and energy indicators have a decisive influence on the expected results of processes carried out in water-salt systems. At present, all known information about the radii and specific energy indicators of atoms and ions are contained in different reference books, which significantly differ from each other. The main reason for the difference is mainly the fact that all the information has been obtained as a result of experimental and indirect research methods; for this reason, the data do not fully correspond to reality. Therefore, using them, it is impossible to consistently and reliably determine the patterns of compositional, phase, structural, and physicochemical changes occurring in water-salt systems. Thus, to consider new possibilities for determining the true values of atom and ion radii as well as specific energy indicators, the reliability of which is no doubt, to determine compositional, phase, structural and physicochemical properties of water-salt systems, and also identifying regularities of the chemical changes are of great importance. Because of this, the search for new possibilities for determining the radii of atoms and ions, their specific energy indicators, the reliability and truth of which is beyond doubt, the establishment of patterns of changes in the composition, structure and physicochemical properties of water-salt systems, the determination of the applied significance of the latest results achieved in this case in relation to the neutralization, utilization by halurgic methods of new, non-natural mineral-salt compositions, which are the inevitable consequences of the practical activities of numerous industrial enterprises, and, today, which are accumulated in the natural environment in quite large quantities are particularly relevant problems of our time.

Relation to research and government programs: The work was carried out in accordance with the plan of the section "Determining the dependence of the physical

and chemical properties of water-salt mixtures on the specific energy indicators of ions" of the state budget topic B-16-02-03 "Development of new technologies for the production of complex fertilizers based on waste from phosphorous and coal production".

Research objects:

- orbital radii, specific energy parameters of atoms and ions of the elements of the D.I. Mendeleev periodic table, their influence on compositional, phase, structural, and physicochemical changes in water-salt systems;
- energy of crystal lattices of mineral salts, its values for chlorides, fluorides, bromides, and iodides;
- influence of the salts' crystal lattice energy on physical and chemical changes in water-salt systems;
- concentration changes in water-salt systems;
- viscosity changes in water-salt systems;
- changes in thermal conductivity in water-salt systems;
- changes in heat capacity in water-salt systems;
- changes in the composition of water-salt systems;
- changes in the phase state of water-salt systems;
- structural changes in water-salt systems;
- applied significance of the research results for halurgy;
- salt production technology of clean productive of salts from the salt waste.

Research purpose and tasks.

- development of science-based methods for calculating the true orbital radii of atoms and ions, determination of specific energy indicators and crystal lattice energy of elementary particles and some mineral salts;
- evaluation of the reliability of the results obtained;
- determination of the influence of newly identified atomic and ionic radii, specific energy indicators, and the mineral salts' crystal lattice energy on the changes in the compositional, phase, structural and physicochemical properties of water-salt systems;
- development of recommendations for their implementation in practice and determining the importance of their use in the halurgic technologies for utilization and neutralization of technogenic wastes in the environment in the form of new modifications of mineral impurities, which are the inevitable consequences of modern production activities;
- development and presentation of technology for the production of pure salts from the production of salt-containing waste by the halurgic method.

Scientific novelty of the research:

- new scientifically sound methods for determining the atomic and ionic radii were developed; the values of atomic and ionic radii as well as specific energy parameters of the elements of the periodic table were determined; their influence

on the regularities of compositional, phase, structural and physicochemical changes in water-salt systems was identified;

- a new method for determining the mineral salts' crystal lattice energy was developed; its application allowed us to calculate values of the crystal lattice energy for representatives of chlorides, iodides, bromides, fluorides often used in modern salt processes; new scientific conclusions about their effect on physicochemical changes in water-salt systems were developed;
- the applied significance of the data obtained during the research is determined;
- the quantitative and qualitative description of the compositional, phase and structural properties of water-salt systems was implemented based on the diagram of a NaCl-H₂O system;
- the technology of production of pure productive sodium chloride from halite waste by halurgic method has been developed, its regime and output indicators in relation to 1 ton of raw materials have been determined.

The main concepts suggested to the defense:

- new approaches for calculating the orbital radii of atoms and ions were developed; using these approaches, the atomic and ionic orbital radii of known chemical elements were determined;
- the specific energy parameters of ions;
- a new method for calculating the mineral salts' crystal lattice energy was developed that allowed us to determine values of the crystal lattice energy of some chlorides, iodides, bromides, fluorides, which are often applied in modern salt processes;
- the influence of the salts' crystal lattice energy on the patterns of physical and chemical changes in water-salt systems was established;
- based on the diagram of a NaCl-H₂O system, the compositional, phase and structural properties of water-salt systems were described quantitatively and qualitatively;
- on the basis of the results of the study, important theoretical and applied conclusions were drawn;
- technology of production of pure product sodium chloride from halite waste by halurgic method.

The research results reliability and approbation. The reliability of the results obtained is guaranteed by application of modern research techniques and confirmed by the analysis of scientific and technical literature and research methods and the preliminary experimental study based on the principles of water-salt systems theory.

Testing the work. The materials of the dissertation work were presented and discussed at various international and national conferences and symposiums: International scientific and practical conference "Actual problems of modern science and education and trends in innovation", dedicated to the 60th anniversary of Professor T.A. Turmambekov, Turkestan, 2017; International scientific and practical conference "Auezov readings – 15": "Third modernization of Kazakhstan – New concepts and

modern solutions”, dedicated to the 120th anniversary of Mukhtar Auezov, 2017; International scientific and practical conference “Conduct of modern science – 2018”, Sheffield, 2018; International scientific and practical conference “Trends and prospects for the development of science and education in the context of globalization”, Pereyaslav-Khmelnytsky, 2018; International scientific and practical conference “Wykształcenie I nauka bez granic – 2018”, Przemysl, Poland, 2018; International scientific and practical conference “Auezov readings – 17: Third modernization of Kazakhstan – New concepts and modern solutions”, Shymkent, 2019.

The personal contribution of the doctoral student includes analyzing the literature on the topic of the dissertation research, choosing the research and analysis techniques, carrying out the experiments, mathematical processing of the research results, and scientific generalization of the results obtained.

Publication of the research results: The main results of the dissertation research were published in 22 publications, including 1 article in journal “EurAsian Journal of Bio Sciences” (Turkey) cited in the Scopus database in 2020; 7 articles in the journals recommended by Committee for control in education and science of the Republic of Kazakhstan; 3 publications in proceedings of international scientific conferences; 5 articles in materials of international and republican conferences in the Republic of Kazakhstan; 3 articles in other scientific journals. In addition, 3 certificates on the objects protected by copyright were obtained.

The dissertation structure and volume

The dissertation thesis contains 164 pages of printed text and includes 47 figures and 64 tables. The thesis consists of the following parts: introduction, literature review, research methods, results and their discussion, and references (109 names).