

COMPLEX METHODOLOGY OF THE MULTICOMPONENT SYSTEMS INVESTIGATION

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Designed general algorithm to complex methodology of the salt systems investigation (CMSSI GA) is created for the expenses minimization on each of three offered information level (the database, qualitative and quantitative system description).

The synthesis of two fundamental approaches to study the heterogeneous equilibrium - a topological method of Kurnakov and thermodynamic method of Gibbs, with the possibilities of the modern computer technology have brought about the CMSSI GA realization and the creation of ideologies for the phase diagrams electronic generator and automatic program complex for their studies - "Dif Pro Generator".

It allows by means of computer modeling to conduct the studies of the multicomponent salt systems with the different types of chemical interaction - exchangeable reactions, chemical compounds formation and solid solutions. A tree of phases is built automatically by means of graph theory. It presents the collection of phase single blocks, on which a composition polyhedron is split, united with each other by the adjacency alignment. The calculation of the eutectic features (composition and temperature) is realized with the using of original thermodynamic correlations of Storonkin-Susarev-Martynova.

The electronic generator of the phase diagrams and program complex "Dif Pro Generator" for the first time in the world practice have allowed to get information on the heterogeneous equilibrium in the multicomponent salt systems in several thousand times faster than in the traditional approach, that allows to economy vastly the materials and time.