INTRODUCTION

The crystal structures of most intermetallic compounds can be presented as a 3D frame of the associated nanoclusters—precursors, in some cases containing clusters—spacers in the cavities of a small number of atoms [1–7]. Nano-sized clusters—precursors have a hierarchical structure. Examples of such clusters, consisting of 40–150 atoms and having linear dimensions of 10–20 Å, are multilayered clusters with an internal polyhedron and external shells (for example, the 45-atomic cluster of McKay [2]), as well as suprapolyhedral clusters formed from several coordination polyhedra (for example, 156-atomic clusters from 13 icosahedra (B12)13 [7]).

There is a correlation between the size of the frame-forming nanoclusters—precursors and the size of the voids in the frame, which in the formation of the intermetallic from the melt are completely filled with atoms—spacers. Upon the formation of large voids in the frame, they are filled with small polyhedral clusters, while polyhedral clusters that are different in
composition and structure can be located in the cavities of different sizes.

Icosahedral clusters \( i \cdot B_{12} \) are polyhedral clusters-precursors in all (five) types of crystalline structures of elemental boron \( B \) and the various binary, ternary, and quaternary boron compounds [8–11].

In four framework structures of elemental boron, extra atoms of \( B \) are present, not included in the icosahedra, and which are spacers. In the two most complicated frame structures of \( B_{196} \) and \( B_{333} \), large metal atoms, e.g., Sc (table) can also enter the frame voids.

When studying double boride \( YB_{66} \) [7], clusters-precursors from 13 icosahedra \( (B_{12})_{13} \) were established with a diameter of ~12 Å, whose packaging contains large voids, statistically filled with atoms-spacers of \( Y \) and \( B \) in the ratio of 1:13. Y, Nd, Sm, and Gd–Lu are atoms of \( A \) that may occupy voids in the icosahedral 3D frame [8, 10]. In the systems with larger atoms \( A = \operatorname{La}, \operatorname{Ce}, \operatorname{Pr}, \) and \( \operatorname{Eu} \) of the first boron-enriched phase is a skeleton compound of \( \text{CaB}_6 \) (\( cP7 \)) type, and this family includes borides with \( A = Y, \operatorname{Er}, \operatorname{Gd}, \operatorname{Th}, \operatorname{Pu}, \operatorname{Nd}, \operatorname{Sm}, \operatorname{Ce}, \operatorname{Yb}, \operatorname{Ca}, \operatorname{La}, \operatorname{Eu}, \operatorname{Sr}, \operatorname{K}, \) and \( \operatorname{Ba} \) [8, 10].

Modern computer techniques [2] allow automatically performing geometric and topological analyses of the chemical compounds of any complexity and detachment nano-sized clusters, corresponding to different levels of the cluster self-organization of chemical systems. In the database created by us more than 200 borides with icosahedral clusters of \( i \cdot B_{12} \) are found; using the ToposPro program package [2], a search for crystal structures containing local areas in the form of clusters from 13 icosahedra \( (B_{12})_{13} \) has been carried out. Among the compounds, containing clusters of \( (B_{12})_{13} \), borides with a different number of atoms in the unit cell are the most crystallochemically difficult: \( \text{ScB}_{13.7} \) \( (oP532) \) [12], \( \text{ScB}_{13.7} \) \( (oP544) \) [13], and \( \text{Sc}_{4.4} \text{Si}_{0.02} \text{B}_{56.4} \text{C}_{3.1} \) \( (oP520) \) [14]. The assumption of the invariance of clusters-precursors from 13 icosahedra of \( (B_{12})_{13} \) for \( \text{ScB}_{13.7} \) and \( YB_{66} \) allows determining at what stage of the self-assembly of the crystal structure from nanoclusters-precursors of \( S_0 \) in the form primary chain \( S_1 \rightarrow \) microlayer \( S_2 \rightarrow \) microframe \( S_3 \) an irreversible evolution of the crystal-forming structural units in the chemical system takes place and revealing the functional role of non-cluster atoms of \( Sc \) and \( B \).

The work continues studies [1–7, 15–17] in the field of the geometric and topological analysis of the structure of crystalline phases, as well as modeling the self-organization processes of chemical systems using modern computer techniques [2, 17].

**TECHNIQUES USED IN COMPUTER ANALYSIS**

The geometric and topological analyses were performed using the ToposPro software complex [2], which allows conducting a multipurpose investigation of the crystal structure in automatic mode, using the representation of the structures in the form of “folded graphs” (factor-graphs). The data on the functional role of atoms in the formation of crystal structures are obtained by the calculation of topological indices (coordination sequences, dot and vertex symbols).