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Crystal structure of $R_3Si_{1.75}Se_7$ (R – 1.5 Y + 1.5 La)

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Abstract

The existence of the new quaternary compound $R_3Si_{1.75}Se_7$ (R – 1.5 Y + 1.5 La) was established. Its crystal structure was studied by X-ray powder method (space group $P6_3$, Pearson symbol hP24-1.44, a = 1.05968(2) nm, c = 0.59995(2) nm, R_I = 0.0414). Rare-earth atoms in the structure of this compound are localized in trigonal prisms with two additional atoms, Si^{IV} atoms center tetrahedra, and Si^{II} atoms lie in octahedra. Quantum chemical simulation of separate fragments of the structure of this mixed selenosilicate (II, IV) was performed.

Keywords: Chalcogenides; Rare earth compounds; Crystal structure; X-ray powder diffraction; Quantum chemical simulation.

1. Introduction

Scientific and technological progress favours the constant search for new materials that meet the requirements of modern technology. One of the main directions of such a search is obtaining compounds by increasing the number of components in their composition, such as ternary and quaternary. The study of multicomponent systems is also an important step in shaping the database of information about new materials. An important place among the multicomponent systems that are intensely studied is occupied by the systems which include chalcogenides of rare earth (RE) metals. The study of the nature of the component interaction in complex RE-containing chalcogenide systems and the study of the crystal structure of the formed compounds is the basis for the creation of new materials with qualitatively new physico-chemical characteristics [1], [2].

The application of a quantum-chemical cluster approach to the simulation of electronic structure, chemical bonding and thermodynamic characteristics in solids makes it possible to study the near-order in the arrangement of atoms in real crystals. A fragment in a cluster model is either simply "cut" out of the

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