NEW APPROACHES IN XRD STUDIES OF MINERALS

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Some exciting recent developments in the field of mineralogical crystallography are considered. The crystal chemical phenomena (e.g. ionic ordering, polyhedral stacking variations, micro-twinning etc.), which accompany the formation of real structures, are discussed on the basis of structural studies of a large group of minerals. The new approaches used for their investigation allow to extend the scientific ideas connected with: status of new and questionable minerals, structural classification of minerals, forms of concentration of chemical elements in the Earth's crust, further development of modular theory and other problems of modern structural mineralogy.

The advantage of using of synchrotron radiation opens the gate to a new branch of microgeochemistry (about 20% of known minerals lack a structure determination, mainly because crystals are too small or imperfect for laboratory X-ray sources). As an example the structures of three arsenates are considered. Two of them are Cu-arsenates, namely zdenekite, $NaPbCu_5(AsO_4)_4Cl{\cdot}5H_2O$ and mahnertite, $(Na,Ca)Cu_3[AsO_4]_2{\cdot}Cl{\cdot}5H_2O$, contain the new type of mixed polyhedral sheets which are characterized by the different mode of their stacking. The specific feature of these layers are the clusters, formed by four $Cu\phi_5$ pyramids (ϕ=O, Cl, H_2O) with shared edges. Zdenekite belongs to mineralogical group of lavendulan, $NaCaCu_5(AsO_4)_4Cl{\cdot}5H_2O$, which also includes sampleite $NaCaCu_5(PO_4)_4Cl{\cdot}5H_2O$. Until recently, none of the representatives of the lavendulan group have been structurally studied.

Tillmannsite, $(Ag_3Hg)(V,As)O_4$, was found in the old copper mines of Roua (Alpes-Maritimes, France) and its structure is characterized by the presence of two types of tetrahedra: metallic clusters formed by Ag and Hg atoms and As,V-tetrahedra. Similar metallic clusters were revealed by WEIL et al. (2005) in the crystal structures of synthetic Ag, Hg-vanadates and arsenates.

The chemical composition of biraite-(Ce), $Ce_2Fe^{2+}(CO_3)(Si_2O_7)$, which is a new mineral from Siberia with a new structural arrangement, was established as a result of its XRD study, IR-spectroscopy and thermal analysis.The microtwinning model was proposed for calcium catapleiite, $CaZrSi_3O_9{\cdot}2H_2O$, which occurs in syenitic pegmatites of Burpala massif. Orthorhombic symmetry is definitely preferable for this mineral and adequately describes its structure. The crystal structure of armstrongite, $CaZr[Si_6O_{15}].3H_2O$, which was discovered in a granite pegmatite and in alkaline granites of Mongolia, was refined using the Rietveld method. As a result the chemical composition of this mineral was determined.

References

WEIL, M., TILLMANNS, E., PUSHCHAROVSKY, D.YU. (2005). Inorg. Chem., 44, 1443-1451.