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Investigation of thermal behavior of mixed-valent iron borates vonsenite and hulsite containing $[OM4]^{n+}$and $[OM\ 5]^{n+}$oxocentred polyhedra by in situ high-temperature Mössbauer spectroscopy, X-ray diffraction and thermal analysis

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Abstract

© 2020 International Union of Crystallography. The investigation of elemental composition, crystal structure and thermal behavior of vonsenite and hulsite from the Titovskoe boron deposit in Russia is reported. The structures of the borates are described in terms of cation-centered and oxocentred polyhedra. There are different sequences of double chains and layers consisting of oxocentred [OM 4] n+ tetrahedra and [OM 5] n+ tetragonal pyramids forming a framework. Elemental composition was determined by energy-dispersive X-ray spectroscopy (EDX). Oxidation states and coordination sites of iron and tin in the oxoborates are determined using Mössbauer spectroscopy and compared with EDX and X-ray diffraction data (XRD). According to results obtained from high-temperature Mössbauer spectroscopy, the Fe2+ to Fe3+ oxidation in vonsenite and hulsite occurs at approximately 500 and 600 K, respectively. According to the high-temperature XRD data, this process is accompanied by an assumed deformation of crystal structures and subsequent solid-phase decomposition to hematite and warwickite. It is seen as a monotonic decrease of volume thermal expansion coefficients with an increase in temperature. A partial magnetic ordering in hulsite is observed for the first time with T c ≃ 383 K. Near this temperature, an unusual change of thermal expansion coefficients is revealed. Vonsenite starts to melt at 1571 K and hulsite melts at 1504 K. Eigenvalues of thermal expansion tensor are calculated for the oxoborates as well as anisotropy of the expansion is described in comparison with their crystal structures.

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Keywords

high-temperature Mössbauer spectroscopy, high-temperature X-ray diffraction, oxidation, oxoborate, thermal expansion

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