Crystal Chemistry and Thermal Expansion of $Mg_{0.5}Zr_2(PO_4)_3$

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Framework phosphates with $Sc_2(WO_4)_3$ (SW) type structures, due to their structural pecularities and a wide variety of iso- and heterovalent chemical substitutions at all crystallographic positions of the structure, allow for the preparation of a large number of closely related compounds and for the selection of SW-compositions to create new materials with desired properties.

Selected results of complex investigations of thermophysical properties (thermal expansion, thermal conductivity, and heat capacity) of the phosphate $Mg_{0.5}Zr_2(PO_4)_3$ are presented. The phosphate crystallizes in an SW structure in the P21/n space group. The thermal expansion behavior of the compound was investigated by high-temperature X-ray powder diffractometry. The thermal expansion coefficients were determined between room temperature and 1023 K. They vary from $-3 \cdot 10^{-6}$ to $7 \cdot 10^{-6}$ K^{-1}. The observed axial thermal expansion and contraction behavior is explained on the basis of the crystal chemistry of the SW family of compounds.