

Lattice thermal expansion of zircon-type LuPO₄ and LuVO₄: A comparative study

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ABSTRACT

We report the lattice thermal expansion of zircon-(xenotime-)type LuPO₄ and LuVO₄ in the temperature range of 25–1000 °C from high-temperature powder XRD studies. The details of the high-temperature crystal chemistry of both phases have been determined from Rietveld analysis of the powder XRD data. Both the compounds show appreciably higher thermal expansion than analogous zircon-type silicates. Despite isomorphism, the axial thermal expansion of LuVO₄ shows significant anisotropy compared to LuPO₄. In the studied temperature range, the average axial thermal expansion coefficients of LuPO₄ are $\alpha_a = 6.0 \times 10^{-6}$ and $\alpha_c = 7.2 \times 10^{-6}$ (°C⁻¹) and those of LuVO₄ are $\alpha_a = 3.6 \times 10^{-6}$ and $\alpha_c = 11.8 \times 10^{-6}$ (°C⁻¹). However, the average volume thermal expansion coefficients are almost identical. The differences in the thermal expansion behavior of the two structures originate from differences in the expansion and distortion of the LuO₈ polyhedra. The LuO₈ polyhedron in LuVO₄ shows about 30% higher thermal expansion than that in LuPO₄. The overall thermal expansion behaviors of these two structures are predominantly related to the distortion in the LuO₈ unit, inter-cation distances and spatial arrangement of the Lu-O bonds in the structure.

Keywords: Thermal expansion, crystal chemistry, zircon, xenotime, phosphates, vanadates