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Structural changes accompanying the phase transformation between leadhillite and susannite: A structural study by means of in situ high-temperature single-crystal X-ray diffraction

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ABSTRACT

To study the temperature-dependent structural changes accompanying the phase transformation leadhillite ↔ susannite and to verify the close structural relationships between heated leadhillite and susannite, a leadhillite crystal has been investigated by X-ray single-crystal diffraction methods within the temperature range 25–100 °C. The values of the unit-cell parameters were determined at 25, 32, 35, 37, 40, 42, 45, 48, 50, 53, 56, 59, 62, 65, 68, 71, 75, 79, 82, 85, 90, 95, and 100 °C. After the heating experiment the crystal was cooled over the same temperature intervals and the unit-cell dimensions were determined again. The values measured with both increasing and decreasing temperature are in excellent agreement, indicating that no hysteresis occurs within the temperature range examined and that the phase transformation is completely reversible in character. Analysis of the components of the spontaneous strain shows only normal thermal expansion up to 50 °C and that the structural distortions leading to the topology of the heated leadhillite take place in the temperature range 50–82 °C. Our study confirms that the crystal structure of heated leadhillite is topologically identical to that of susannite and that the slight structural changes occurring during the phase transformation leadhillite ↔ susannite are mainly restricted to the sulfate sheet. Changes in the orientation of sulfate tetrahedra and in the Pb-O coordination polyhedra occur in a continuous way within the temperature range investigated as indicated by the second-order character of the phase transition. In this way, the leadhillite structure gradually goes toward that of susannite without abrupt structural changes.