

Crystal structures of synthetic melanotekite (Pb₂Fe₂Si₂O₉), kentrolite (Pb₂Mn₂Si₂O₉), and the aluminum analogue (Pb₂Al₂Si₂O₉)

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ABSTRACT

Synthetic crystals of melanotekite and kentrolite were obtained at 850 °C from melt. The aluminum analogue of kentrolite Pb₂Al₂Si₂O₉ was hydrothermally synthesized at 2 GPa, 650 °C together with zoisite-(Pb) and margarite-(Pb). Synthesis products were characterized by single-crystal diffraction studies and microprobe analysis.

The aluminum analogue Pb₂Al₂Si₂O₉ was observed in space group *Pbcn* with lattice parameters $a = 6.8981(7) \text{ \AA}$, $b = 10.6906(15) \text{ \AA}$, $c = 9.7413(10) \text{ \AA}$, and $V = 718.37 \text{ \AA}^3$. Fourier mappings show no irregularities of the Pb site.

Melanotekite with lattice parameters $a = 6.9786(6) \text{ \AA}$, $b = 11.0170(11) \text{ \AA}$, $c = 10.0895(9) \text{ \AA}$, and $V = 775.71(17) \text{ \AA}^3$ in space group *Pbcn* show a slightly deformed Pb-position in Fourier mappings.

Kentrolite was observed in space group *P2₁2₂1* with pseudo-symmetry to *Pbcn* with lattice parameters $a = 7.0103(5) \text{ \AA}$, $b = 11.0729(7) \text{ \AA}$, $c = 9.9642(7) \text{ \AA}$, and $V = 773.47(11) \text{ \AA}^3$. Fourier mappings of the kentrolite structure show that two different split Pb sites exist, which causes lower symmetry. The unit-cell volume of different members of the kentrolite group is a linear function of trivalent ionic radii in sixfold coordination for the elements Al, Ga, In, and also for Fe and Mn in high spin mode.

The structure of Pb₂M₂Si₂O₉ (M = Al³⁺, Fe³⁺, Mn³⁺) is built on isolated M-octahedra chains parallel *c*, M-octahedra sharing alternately *trans* and *skew* edges. Each Si₂O₇-group is linked with their vertices to three octahedra chains. Their Si-O-Si bond angles depend on the size of M-octahedra and are 129.84° in Pb₂Al₂Si₂O₉, 131.08° in Pb₂Fe₂Si₂O₉, 128.34° and 130.33° in Pb₂Mn₂Si₂O₉.

Keywords: Kentrolite, melanotekite, Pb₂Al₂Si₂O₉, Pb₂Fe₂Si₂O₉, Pb₂Mn₂Si₂O₉, crystal-structure, X-ray-diffraction, EMP-analysis