American Mineralogist, Volume 93, pages 573–583, 2008

Crystal structures of synthetic melanotekite ($Pb_2Fe_2Si_2O_9$), kentrolite ($Pb_2Mn_2Si_2O_9$), and the aluminum analogue ($Pb_2Al_2Si_2O_9$)

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Abstract

Synthetic crystals of melanotekite and kentrolite were obtained at 850 °C from melt. The aluminum analogue of kentrolite $Pb_2Al_2Si_2O_9$ 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 $Pb_2Al_2Si_2O_9$ was observed in space group *Pbcn* with lattice parameters $a = 6.8981(7)$ Å, $b = 10.6906(15)$ Å, $c = 9.7413(10)$ Å, and $V = 718.37$ Å^3. Fourier mappings show no irregularities of the Pb site.

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

Kentrolite was observed in space group $P2_122_1$ with pseudo-symmetry to *Pbcn* with lattice parameters $a = 7.0103(5)$ Å, $b = 11.0729$ (7) Å, $c = 9.9642(7)$ Å, and $V = 773.47(11)$ Å^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 $Pb_2M_2Si_2O_9$ ($M = Al^{3+}$, Fe^{3+}, Mn^{3+}) is built on isolated M-octahedra chains parallel **c**, M-octahedra sharing alternately *trans* and *skew* edges. Each Si_2O_7-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 $Pb_2Al_2Si_2O_9$, 131.08° in $Pb_2Fe_2Si_2O_9$, 128.34° and 130.33° in $Pb_2Mn_2Si_2O_9$.

Keywords: Kentrolite, melanotekite, $Pb_2Al_2Si_2O_9$, $Pb_2Fe_2Si_2O_9$, $Pb_2Mn_2Si_2O_9$, crystal-structure, X-ray-diffraction, EMP-analysis