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The crystal structure of a second antigorite polysome (m = 16), by single-crystal synchrotron diffraction

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ABSTRACT

A model for the modulated crystal structure of an antigorite polysome with m = 16 (where m is related to the number of tetrahedra spanning a wavelength along **a**) was refined by single-crystal synchrotron diffraction data in $C2/m$, using crystals coexisting with the m = 17 polysome from Val Malenco, Italy, which was previously determined structurally. Lattice parameters [a = 81.664(10), b = 9.255(5), c = 7.261(5) Å, β = 91.409(5)°] were determined using a single-crystal diffractometer equipped with an area detector at the Desy synchrotron (Hamburg). The structure was solved by direct methods, and the model refined using 19 222 symmetry-related reflections. The final $R_{4\sigma}$ factor was 0.0951, calculated for 7246 reflections.

The structure of the m = 16 antigorite polysome strongly resembles that of the m = 17 polysome. A continuous, wavy octahedral sheet is linked to a tetrahedral sheet, reversing its polarity through sixfold tetrahedral and eightfold tetrahedral rings. The half-wave has a curvature radius of 80.1 Å. Polyhedral geometry, ditrigonalization angles, and interlayer O-O distances are similar in the two polysomes. The only differences concern the number of tetrahedra for the m = 16 polysome (an even number which leads to symmetric half-waves) and the periodic **b**/2 shift involving the eightfold rings (to produce the doubling of the a parameter and a C-centered cell).

Keywords: Antigorite, structure, synchrotron, polysomatism