The modulated crystal structure of antigorite: The m = 17 polysome GIANCARLO CAPITANI* AND MARCELLO MELLINI

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ABSTRACT

The modulated crystal structure of an antigorite polysome with m=17 was refined by single crystal X-ray diffraction in the Pm space group, using highly ordered single crystals from Val Malenco, Italy. The chemical composition is $(Mg_{2.673}Fe_{0.098}^{2.673}Fe_{0.098}^{2.673}Fe_{0.003}^{3.610}Al_{0.035}Cr_{0.007}Ni_{0.003}Mn_{0.002})_{\Sigma=2.823}(Si_{1.997}Al_{0.003})_{\Sigma=2}O_5(OH)_{3.639}$.

Lattice parameters [a = 43.505(6), b = 9.251(1), c = 7.263(1) Å, $\beta = 91.32(1)^{\circ}$] were determined using a single-crystal diffractometer equipped with an area detector. The structure was refined using 9242 independent reflections, obtaining a final $R_{4\sigma}$ factor of 0.0577. A continuous, wavy octahedral sheet is linked to a tetrahedral sheet with tetrahedral apices alternatively pointing +c and -c. This sheet is located on the concave side of the octahedral-sheet wave. The octahedral sheet shows normal thickness for a serpentine of this composition, and does not have any internal offset. The tetrahedral sheet inverts its polarity through six- and eight-membered tetrahedral rings (6- and 8-reversals). Between reversals, 6-membered rings are distorted toward ditrigonal configuration, with tetrahedral rotation, α values, ranging along the wave from 4 to 13.6°. The two half-waves have curvature radii of 99.4 and 110.9 Å. Variable interlayer O-O distances occur, indicating the absence of homogeneous, continuous hydrogen bonding. The bond geometry, very similar to that of lizardite, suggests common crystal chemical and geochemical properties. The larger stability field of antigorite compared to lizardite is interpreted to arise from the occurrence of three-dimensionally connected chemical bonds.