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Another step toward understanding the true nature of sartorite: Determination and refinement of a ninefold superstructure

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ABSTRACT

Single-crystal X-ray diffraction data, collected from a sartorite crystal from Lengenbach (Binntal, Valais, Switzerland), yielded a ninefold superstructure: space group $P2_1/c$; $a = 37.71(2)$, $b = 7.898(3)$, $c = 20.106(8)$ Å, $\beta = 101.993(7)°$; $R_1 = 6.08\%$ for 6293 reflections with $I > 2\sigma_I$. The sample is an $N_{1,2} = 3,3$ sartorite homologue and the refined formula $Pb_8Tl_{1.5}As_{17.5}S_{35}$ compares very well with the empirical formula $Pb_{8.2}Tl_{1.4}As_{17.5}Sb_{0.5}S_{35}$ obtained from electron microprobe analyses. It has a high Tl content, up to 6.5 wt%. In a coupled substitution approximately 1.5 Tl^+ replace about 0.5 As^{3+} and 1 PbS. The refined structure has 35 S atoms pfu instead of the expected 36 S (= 9 × 4 S, from $PbAs_2S_4$). The incorporation of substantial amounts of Tl^+ into $PbAs_2S_4$ is essential for the type and periodicity of superstructures in sartorite. The refined superstructure can be interpreted as a so-called "lock-in" structure with a composition that yields a commensurate lattice for a mineral that usually has an incommensurate lattice. No commensurate periodicity could be found for a second crystal with about 0.5 Tl apfu.