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Fettelite, $[Ag_6As_2S_7][Ag_{10}HgAs_2S_8]$ from Chañarcillo, Chile: Crystal structure, pseudosymmetry, twinning, and revised chemical formula

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Abstract

The crystal structure of the rare mineral fettelite was solved using intensity data collected from a twinned crystal from Chañarcillo, Copiapó Province, Chile. This study revealed that, in spite of the strong hexagonal pseudosymmetry, the structure is monoclinic (space group $C2$) with $a = 26.0388(10)$, $b = 15.0651(8)$, $c = 15.5361(8)$ Å, $\beta = 90.48(1)°$, and $V = 6094.2(5)$ Å^3. The refinement of an anisotropic model led to an R index of 0.0656 for 7143 observed reflections [$I > 2\sigma(I)$] and 0.0759 for all 17 447 independent reflections. Fettelite is intimately twinned with six twin domains. The structure consists of the stacking of two module layers along [001]: an A module layer with composition $[Ag_6As_2S_7]^{2-}$ and a B module layer with composition $[Ag_{10}HgAs_2S_8]^{2+}$. The As atoms form isolated AsS_3 pyramids typical of sulfosalts, Hg links two sulfur atoms in linear coordination, and Ag occupies sites with coordination ranging from quasi linear to almost tetrahedral. The A module layer found for fettelite is identical to that described for the minerals belonging to the pearceite-polybasite group. On the basis of information gained from this characterization the crystal chemical formula was revised according to the structural results, yielding $[Ag_6As_2S_7][Ag_{10}HgAs_2S_8]$ ($Z = 8$).

Keywords: Silver sulfosalts, crystal structure, chemical composition, optical properties, fettelite, pearceite-polybasite, polytypes, physical properties