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Gillulyite $\text{Tl}_2(\text{As,Sb})_8\text{S}_{13}$: Reinterpretation of the crystal structure and order-disorder phenomena*

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ABSTRACT

The crystal structure of gillulyite $\text{Tl}_2(\text{As, Sb})_8\text{S}_{13}$ was reinterpreted based on the average structure determined by Foit et al. (1995). It consists of alternating PbS-like slabs comprised of As-S polyhedra and Tl-bearing slabs with partly zeolitic properties. In the latter, TlS_5 and As_2S_5 groups alternate regularly along the b direction and across the width of the slab, thus eliminating the need for S-S and As-As bonds postulated by Foit et al. (1995). These two types of slabs are also unit order-disorder (OD) layers, the ambiguities in stacking of which lead to several potential gillulyite polytypes. The actually observed OD phenomena are caused by ambiguity in the position of $[010]$ TlS_5 - As_2S_5 sequences (or of entire such layers), which can with equal probability assume two positions $1b$ apart.