

LETTER

**Crystal structure of argentopyrite,  $\text{AgFe}_2\text{S}_3$ , and its relationship with cubanite**

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ABSTRACT

The structure of argentopyrite,  $\text{AgFe}_2\text{S}_3$ , was determined for the first time with single-crystal X-ray diffraction. In contrast to the previously reported orthorhombic symmetry, our data show that argentopyrite is monoclinic with space group  $P112_1/n$  (non-standard setting) and unit-cell parameters  $a = 6.6902(2)$ ,  $b = 11.4497(4)$ ,  $c = 6.4525(2)$  Å,  $\gamma = 90.2420(8)^\circ$ , and  $V = 494.26(3)$  Å<sup>3</sup>. Similar to cubanite ( $\text{CuFe}_2\text{S}_3$ ), the structure of argentopyrite is also based on approximately hexagonal close-packed S atoms, with cations ordered over one half of the tetrahedral sites, forming corner-shared  $\text{AgS}_4$  and  $\text{FeS}_4$  tetrahedral sheets parallel to (001). The two structures differ chiefly in the linkage between the two adjacent tetrahedral sheets and the ordering patterns of cations within a tetrahedral sheet. Topologically, the structure of argentopyrite can be obtained by a displacement of a tetrahedral sheet in the cubanite structure along the ( $a/2 + b/6$ ) direction relative to the sheet beneath, giving rise to a cluster of *four* edge-shared  $\text{FeS}_4$  tetrahedra in argentopyrite, as compared to *two* in cubanite. There are *two* distinct Fe sites (Fe1 and Fe2) in argentopyrite, rather than only *one*, as in other  $\text{MFe}_2\text{S}_3$  sulfide minerals (M = monovalent cations). Together with published Mössbauer data, we suggest that there exists some degree of  $\text{Fe}^{2+}$ - $\text{Fe}^{3+}$  order-disorder in argentopyrite, with  $\text{Fe}^{2+}$  favoring the more distorted Fe2 tetrahedral site. Argentopyrite appears to possess all the features proposed by Putnis (1977) for a high-temperature ordered form of cubanite.

**Keywords:** Argentopyrite,  $\text{AgFe}_2\text{S}_3$ , Ag-Fe sulfides, cubanite-related mineral, sternbergite, crystal structure, single-crystal X-ray diffraction