

Superstructure, crystal chemistry, and cation distribution in filipstadite, a Sb⁵⁺-bearing, spinel-related mineral

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ABSTRACT

The crystal structure of the rare, spinel-related Sb mineral filipstadite from Långban, Filipstad district, Värmland, Sweden, has been solved and refined in the space group $Fd\bar{3}m$ [$a = 25.9300(6)$ Å, $V = 17434.4(5)$ Å³, and $Z = 216$] and refined to $R = 4.41\%$ for 681 $F_o > 4\sigma(F_o)$ using MoK α X-ray data. The structure of filipstadite is topologically identical to the spinel-type structure with cations occupying 1/8 of the tetrahedral (T) and 1/2 of the octahedral (M) interstices of a cubic close-packing of oxygen atoms. Due to the cation ordering, which leads to the tripling of the unit-cell edge, the M and T sites of the spinel-type structure split into six and five independent sites, respectively. Chemical composition was determined by electron microprobe. The fractions of major cations obtained from chemical analysis were distributed between T and M sites taking into account the weighted electron number at both T and M sites, and minimizing the discrepancy between the calculated and the observed overall <M-O> distance. Cations present in minor amounts were assigned on the basis of their known site preference. The obtained populations ($2M = \text{Mn}_{0.56}^{2+}\text{Mg}_{0.76}\text{Fe}_{0.16}^{3+}\text{Al}_{0.02}\text{Sb}_{0.50}^{5+}$; $T = \text{Mn}_{0.60}^{2+}\text{Mg}_{0.07}\text{Fe}_{0.30}^{3+}\text{Zn}_{0.02}\text{Si}_{0.01}^{4+}$) were then tentatively distributed among the individual M and T sites on the basis of crystal chemical considerations.

Keywords: Filipstadite, spinel, crystal structure determination, superstructure, cation distribution, Långban (Sweden)