

Crystal chemistry of Bi- and Mn-bearing vesuvianite from Långban, Sweden

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ABSTRACT

Red vesuvianite crystals occur with hausmanite and calcite in a hand specimen from Långban, Sweden. Backscattered electron imaging revealed that a very few of the vesuvianite crystals exhibit cores of higher average atomic number (vesuvianite I) than the bulk (vesuvianite II). Average electron microprobe compositions of vesuvianite I show 3.32 wt% MnO (1.43 Mn²⁺ apfu), 3.13 wt% Bi₂O₃ (0.41 Bi³⁺ apfu), 0.82 wt% Cl (0.71 Cl apfu), and 0.56 wt% As₂O₅ (0.15 As⁵⁺ apfu). The average vesuvianite II composition shows considerably more Mn (4.14 wt% MnO, or 1.76 Mn²⁺ apfu) but less Bi (0.62 wt% Bi₂O₃, or 0.08 Bi³⁺ apfu) and Cl (0.13 wt% Cl, or 0.11 Cl apfu) and about the same amount of As (0.62 wt% As₂O₅, or 0.16 As⁵⁺ apfu). The crystal structures of vesuvianite I ($a = 15.595$, $c = 11.779$ Å) and II ($a = 15.585$, $c = 11.778$ Å) were refined in space group $P4/nnc$ to R_1 values of 0.0445 and 0.0167, respectively. The results show Bi at the new Bi3 position and Cl at the new Cl site; Bi3 can only be occupied when there is a vacancy at the nearby (~0.4 Å) X3 position, and Cl when there is a vacancy at the nearby (~0.4–0.5 Å) O10 position. Bond distances and site occupancies suggest that the Cl atom at the Cl site is bonded to the Bi atom at the Bi3 position when it is occupied. Arsenic occupies the T1 site and is coordinated by oxygen atoms at two O7B and two O11 positions. Manganese replaces Ca at the X1 and X2 position and dominates the Y1 position in vesuvianite I, whereas in vesuvianite II it replaces Ca at the X1 site and fills the Y1A position. In both structures Mn also occurs subordinate to Al + Mg at the Y3 position. Bond-valence analysis indicates that the Mn at the Y1 and Y1A positions is divalent rather than trivalent as required for manganvesuvianite.

Keywords: Vesuvianite, Långban, manganese, bismuth, arsenic, crystal structure