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SPECIAL COLLECTION: APATITE: A COMMON MINERAL, UNCOMMONLY VERSATILE

The crystal structure of svabite, $Ca_5(AsO_4)_3F$, an arsenate member of the apatite supergroup

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Abstract

The crystal structure of svabite, ideally $Ca_5(AsO_4)_3F$, was studied using a specimen from the Jakobsberg mine, Värmland, Sweden, by means of single-crystal X-ray diffraction data. The structure was refined to $R_1 = 0.032$ on the basis of 928 unique reflections with $F_o > 4\sigma(F_o)$ in the $P6_3/m$ space group, with unit-cell parameters $a = 9.7268(5)$, $c = 6.9820(4)$ Å, $V = 572.07(5)$ Å^3. The chemical composition of the sample, determined by electron-microprobe analysis, is (in wt%, average of 10 spot analyses): SO_3 0.49, P_2O_5 0.21, V_2O_5 0.04, As_2O_5 51.21, SiO_2 0.19, CaO 39.31, MnO 0.48, SrO 0.03, PbO 5.19, Na_2O 0.13, F 2.12, Cl 0.08, H_2O_{calc} 0.33, O (≡ F+Cl) –0.91, total 98.90. On the basis of 13 anions per formula unit, the empirical formula corresponds to $(Ca_{4.66}Pb_{0.16}Mn_{0.04}Na_{0.03})_{\Sigma 4.89}(As_{2.96}S_{0.04}Si_{0.02}P_{0.02})_{\Sigma 3.04}O_{12}[F_{0.74}(OH)_{0.24}Cl_{0.01}]$. Svabite is topologically similar to the other members of the apatite supergroup: columns of face-sharing $M1$ polyhedra running along **c** are connected through TO_4 tetrahedra with channels hosting $M2$ cations and X anions. The crystal structure of synthetic $Ca_5(AsO_4)_3F$ was previously reported as triclinic. On the contrary, the present refinement of the crystal structure of svabite shows no deviations from the hexagonal symmetry. An accurate knowledge of the atomic arrangement of this apatite-remediation mineral represents an improvement in our understanding of minerals able to sequester and stabilize heavy metals such as arsenic in polluted areas.

Keywords: Svabite, calcium arsenate, apatite supergroup, crystal structure, Jakobsberg mine, Sweden