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SPECIAL COLLECTION: APATITE: A COMMON MINERAL, UNCOMMONLY VERSATILE

The crystal structure of turneaureite, $Ca_5(AsO_4)_3Cl$, the arsenate analog of chlorapatite, and its relationships with the arsenate apatites johnbaumite and svabite

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Abstract

The crystal structure of turneaureite, ideally $Ca_5(AsO_4)_3Cl$, was studied using a specimen from the Brattfors mine, Nordmark, Värmland, Sweden, by means of single-crystal X-ray diffraction data. The structure was refined to $R_1 = 0.017$ on the basis of 716 unique reflections with $F_o > 4\sigma(F_o)$ in the $P6_3/m$ space group, with unit-cell parameters $a = 9.9218(3)$, $c = 6.8638(2)$ Å, $V = 585.16(4)$ Å^3. The chemical composition of the sample, determined by electron-microprobe analysis, is (in wt%; average of 10 spot analyses): SO_3 0.22, P_2O_5 0.20, V_2O_5 0.01, As_2O_5 51.76, SiO_2 0.06, CaO 41.39, MnO 1.89, SrO 0.12, BaO 0.52, PbO 0.10, Na_2O 0.02, F 0.32, Cl 2.56, H_2O_{calc} 0.58, O(≡F+Cl) –0.71, total 99.04. On the basis of 13 anions per formula unit, the empirical formula corresponds to $(Ca_{4.82}Mn_{0.17}Ba_{0.02}Sr_{0.01})_{\Sigma 5.02}(As_{2.94}P_{0.02}S_{0.02}Si_{0.01})_{\Sigma 2.99}O_{12}[Cl_{0.47}(OH)_{0.42}F_{0.11}]_{\Sigma 1.00}$.

Turneaureite is topologically similar to the other members of the apatite supergroup: columns of face-sharing *M*1 polyhedra running along **c** are connected through TO_4 tetrahedra with channels hosting *M*2 cations and *X* anions. Owing to its particular chemical composition, the studied turneaureite can be considered as a ternary calcium arsenate apatite; consequently it has several partially filled anion sites within the anion columns. Polarized single-crystal FTIR spectra of the studied sample indicate stronger hydrogen bonding and less diverse short-range atom arrangements around (OH) groups in turneaureite as compared to the related minerals johnbaumite and svabite. 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: Turneaureite, calcium arsenate, apatite supergroup, crystal structure, infrared spectroscopy, Sweden, Apatite: A common mineral, uncommonly versatile