Phosphovanadylite: A new vanadium phosphate mineral with a zeolite-type structure

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Abstract

Phosphovanadylite, whose simplified formula is $(Ba,Ca,K,Na)_{*}[(V,Al)_{4}P_{2}(O,OH)_{16}]$ ·12H₂O, is a new vanadium phosphate zeolite mineral found in the Phosphoria Formation at Monsanto's Enoch Valley Mine, Soda Springs, Idaho. Its formula in more detail is $(Ba_{0.38}Ca_{0.20}K_{0.06}Na_{0.02})_{\Sigma 0.66}[P_{2}(V_{3.44}Al_{0.46})_{\Sigma 3.90}O_{10.34}(OH)_{5.66}]$ ·12H₂O. The drusy mineral occurs as pale greenish-blue euhedral cubes $(20-50 \ \mu\text{m} \text{ edge})$ coating phosphatic, organic-rich mudstone. The chemical composition determined by electron microprobe is (in weight percent) V-28.02, P-9.91, Al-1.97, Ca-1.31, Ba-8.28, Cd-0.09, Zn-0.34, Na-0.15, K-0.73, O-46.57, and F-0.03. The index of refraction is $n_D = 1.566$ (4) and specific gravity is 2.16 (3). The X-ray powder pattern shows strong reflections at 3.16 Å (422), 2.58 (600), 2.44 (620), and 7.73 (200), which are indexed on the basis of a cubic body-centered unit cell with a = 15.470 (4) Å. From the single-crystal structure analysis, its space group was determined to be $I\overline{43}m$, Z = 6, and its structure consists of V₄O₁₆ octahedral clusters linked to each other by P atoms to form a cubic lattice, creating cavities 7.0 and 5.5 Å in diameter where mainly H₂O resides. Final residual indexes are R = 0.066, $R_w = 0.061$, goodnessof-fit = 0.75, and 93 observations and 24 parameters.