

## Phosphovanadylite-Ca, $\text{Ca}[\text{V}_4^{4+}\text{P}_2\text{O}_8(\text{OH})_8]\cdot 12\text{H}_2\text{O}$ , the Ca analogue of phosphovanadylite-Ba

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### ABSTRACT

Phosphovanadylite-Ca,  $\text{Ca}[\text{V}_4^{4+}\text{P}_2\text{O}_8(\text{OH})_8]\cdot 12\text{H}_2\text{O}$ , is a new mineral from the South Rasmussen (or South Rasmussen Ridge) phosphate mine, Soda Springs, Caribou County, Idaho. It is named as the Ca analog of phosphovanadylite, which is now renamed as phosphovanadylite-Ba. The new mineral grows on matrix containing fine-grained quartz, massive, porous fluorapatite and hydroxylapatite, framboidal pyrite, and tiny, euhedral sphalerite crystals. Other minerals directly associated with the new mineral are sincosite and native Se. Phosphovanadylite-Ca crystallized at ambient temperatures from late-stage aqueous solutions of near neutral pH under relatively reducing conditions. The mineral is cubic, space group  $\bar{I}43m$ ,  $a = 15.441(11) \text{ \AA}$ ,  $V = 3682(5) \text{ \AA}^3$ , and  $Z = 6$ . Crystals occur as small, greenish-blue simple cubes (to 0.1 mm on edge) intergrown to form thin crusts. Penetration twinning on  $\{111\}$  is common. The color is bright greenish blue, the streak is very pale greenish blue, and the luster is vitreous. The Mohs hardness is estimated at 2. The new mineral is brittle with irregular fracture and no cleavage. The measured density is  $2.02(3) \text{ g/cm}^3$  and the calculated density based on the empirical formula is  $2.038 \text{ g/cm}^3$ . Phosphovanadylite-Ca is isotropic with  $n = 1.559(2)$ . The normalized electron microprobe analysis based upon sufficient H for charge balance and 12 molecules of zeolitic  $\text{H}_2\text{O}$  is:  $\text{Na}_2\text{O}$  0.22,  $\text{K}_2\text{O}$  0.55,  $\text{CaO}$  5.58,  $\text{SrO}$  0.10,  $\text{BaO}$  0.21,  $\text{Al}_2\text{O}_3$  3.27,  $\text{VO}_2$  35.85,  $\text{P}_2\text{O}_5$  18.78,  $\text{H}_2\text{O}$  35.44, Total 100.00. The empirical formula (based on 2 P and 28 O apfu) is:  $(\text{Ca}_{0.75}\text{K}_{0.09}\text{Na}_{0.05}\text{Ba}_{0.01}\text{Sr}_{0.01})_{\Sigma 0.91}[(\text{V}_{3.27}^{4+}\text{Al}_{0.49})_{\Sigma 3.76}\text{P}_{2.00}\text{O}_{10.23}(\text{OH})_{5.77}]\cdot 12\text{H}_2\text{O}$ . The eight strongest powder X-ray diffraction lines are [ $d_{\text{obs}}$  in  $\text{ \AA}$  ( $hkl$ )  $I$ ]: 11.04 (110) 97, 7.7881 (200) 100, 4.487 (222) 14, 3.1706 (422) 46, 2.749 (440) 32, 2.4576 (620) 14, 2.3426 (622) 15, and 1.8295 (822) 16. The crystal structure of phosphovanadylite-Ca ( $R_1 = 0.027$  for 171 reflections with  $F_o > 4\sigma F$ ) contains  $\text{V}_4^{4+}\text{O}_{16}$  polyvanadate clusters of four edge-sharing  $\text{V}^{4+}\text{O}_6$  octahedra. The polyvanadate clusters are linked into a three-dimensional zeolite-like framework by sharing corners with  $\text{PO}_4$  tetrahedra. The open space in the framework is dominated by  $\text{H}_2\text{O}$  with the equivalent of one large cation pfu sharing one of the  $\text{H}_2\text{O}$  sites. The framework is identical to that in phosphovanadylite-Ba; however, in phosphovanadylite-Ba, the dominant extra-framework cation is Ba, while in phosphovanadylite-Ca, it is Ca.

**Keywords:** Phosphovanadylite-Ca, new mineral, crystal structure, zeolite-type structure, phosphovanadylite-Ba, South Rasmussen phosphate mine, Idaho