

## Kapundaite, $(\text{Na,Ca})_2\text{Fe}^{3+}(\text{PO}_4)_4(\text{OH})_3 \cdot 5\text{H}_2\text{O}$ , a new phosphate species from Toms quarry, South Australia: Description and structural relationship to mélonjosephite

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### ABSTRACT

Kapundaite, ideally  $(\text{Na,Ca})_2\text{Fe}^{3+}(\text{PO}_4)_4(\text{OH})_3 \cdot 5\text{H}_2\text{O}$ , is a new mineral (IMA2009-047) from Toms phosphate quarry, Kapunda, South Australia, Australia. The new mineral occurs as cavernous aggregates of fibers up to several centimeters across, associated with leucophosphite, natrodufrenite, and meurigite-Na crystals and amorphous brown, black, and/or greenish coatings. Individual kapundaite crystals are very thin flattened fibers up to a few millimeters in length, but typically no more than a few micrometers in thickness. The main form observed is  $\{100\}$ ; other forms in the  $[010]$  zone are present, but cannot be measured. Crystals of kapundaite are pale to golden yellow, transparent to translucent, have a yellow streak and silky luster, and are non-fluorescent. Mohs hardness is estimated to be about 3; no twinning or cleavage was observed. Kapundaite is biaxial (+), with indices of refraction  $\alpha = 1.717(3)$ ,  $\beta = 1.737(3)$ , and  $\gamma = 1.790(3)$ .  $2V$  could not be measured;  $2V_{\text{calc}}$  is  $64.7^\circ$ . The optical orientation is  $Z = \mathbf{b}$ ,  $Y \approx \mathbf{c}$  with weak pleochroism:  $X =$  nearly colorless,  $Y =$  light brown,  $Z =$  pale brown; absorption:  $Y > Z > X$ . No dispersion was observed. The empirical chemical formula (mean of seven electron microprobe analyses) calculated on the basis of 24 O is  $(\text{Ca}_{1.13}\text{Na}_{0.95})_{\Sigma 2.08}(\text{Fe}_{3.83}^{3+}\text{Mn}_{0.03}\text{Al}_{0.02}\text{Mg}_{0.01})_{\Sigma 3.89}\text{P}_{3.92}\text{O}_{16}(\text{OH})_3 \cdot 5\text{H}_{2.11}\text{O}$ . Kapundaite is triclinic, space group  $P\bar{1}$ ,  $a = 6.317(5)$ ,  $b = 7.698(6)$ ,  $c = 9.768(7)$  Å,  $\alpha = 105.53(1)^\circ$ ,  $\beta = 99.24(2)^\circ$ ,  $\gamma = 90.09(2)^\circ$ ,  $V = 451.2(6)$  Å<sup>3</sup>, and  $Z = 1$ . The five strongest lines in the powder X-ray diffraction pattern are [ $d_{\text{obs}}$  in Å ( $hkl$ ): 9.338 (100) (001), 2.753 (64) ( $2\bar{1}1$ ), 5.173 (52) (011), 2.417 (48) ( $2\bar{1}3$ , 202,  $0\bar{1}4$ ), and 3.828 (45) ( $0\bar{2}1$ ). The crystal structure was solved from single-crystal X-ray diffraction data using synchrotron radiation and refined to  $R_1 = 0.1382$  on the basis of 816 unique reflections with  $F_o > 4\sigma F$ . The structure of kapundaite is based on a unique corrugated octahedral-tetrahedral sheet, which is composed of two types of chains parallel to  $\mathbf{a}$ . Kapundaite is structurally related to mélonjosephite. The mineral is named for the nearest town to the quarry.

**Keywords:** Kapundaite, new mineral, phosphate, Toms phosphate quarry, crystal structure, octahedral-tetrahedral sheet, mélonjosephite