

## The crystal structure of johnbaumite, $\text{Ca}_5(\text{AsO}_4)_3\text{OH}$ , the arsenate analogue of hydroxylapatite

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### ABSTRACT

The crystal structure of johnbaumite, ideally  $\text{Ca}_5(\text{AsO}_4)_3\text{OH}$ , was determined and refined using crystals from the Harstigen mine, Värmland, Sweden, on the basis of X-ray diffraction data. The structure was refined to  $R_1 = 0.038$  in space group  $P6_3/m$ , with unit-cell parameters  $a = 9.7242(2)$ ,  $c = 6.9657(9)$  Å, and  $V = 570.43(2)$  Å<sup>3</sup>. The chemical composition of the sample, determined by electron-microprobe analysis, is  $(\text{Ca}_{5.02}\text{Pb}_{0.03})_{\Sigma 5.05}[\text{As}_{2.91}\text{P}_{0.04}\text{Si}_{0.02}]_{\Sigma 2.97}\text{O}_{12}(\text{OH}_{0.97}\text{Cl}_{0.03})$ .

Johnbaumite belongs to the calcium arsenate apatites, together with svabite,  $\text{Ca}_5(\text{AsO}_4)_3\text{F}$ , and turneaureite,  $\text{Ca}_5(\text{AsO}_4)_3\text{Cl}$ . Johnbaumite is topologically similar to the other members of the apatite supergroup: columns of face-sharing  $M1$  polyhedra run along  $c$  and are connected through  $\text{TO}_4$  tetrahedra, giving rise to a zeolite-like microporous framework, with channels hosting  $M2$  cations and  $X$  anions.

This is the first published single-crystal structure study of johnbaumite and the first report of this calcium arsenate apatite from the Harstigen mine. Actually, johnbaumite was identified at this locality at the end of the 19th Century but it was described as svabite.

**Keywords:** Johnbaumite, calcium arsenate, apatite supergroup, crystal structure, Harstigen mine