A POTENTIALLY NEW MINERAL WITH A MODULAR STRUCTURE BASED ON ANTIPEROVSKITE LAYERS

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The potentially new mineral $Ba_2Ca_{18}(SiO_4)_6(PO_4)_3(CO_3)F_3O$ was found in spurrite pyrometamorphic rocks of the Hatrurim Complex in the Negev Desert, near Arad City, Israel, associated with spurrite, calcite, brownmillerite, shulamitite, CO_3-bearing fluorapatite, brucite, fluormayenite-fluorkyuygenite, periclase, barytocalcite, baryte and the recently accepted new minerals ariegilatite $BaCa_{12}(SiO_4)_4(PO_4)_2F_2O$ and stracherite $BaCa_{12}(SiO_4)_2[(PO_4)(CO_3)]F$ (GALUSKIN et al., 2017a, b).

Single-crystal diffraction data was collected using synchrotron radiation (X06DA, Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland). The crystal structure was refined to $R1 = 7.5\%$ (*R-3m*, $a = 7.12546(11)$, $c = 66.2902(13)$ Å, $V = 2914.78(9)$ Å^3, $Z = 3$).

The structure of the 'new' mineral can be described as a stacking of three different modules along (001): six layers of $\{Ba(PO_4)_{1.5}(CO_3)_{0.5}\}^{3.5-}$, three triple antiperovskite (AP) layers $\{(F_2OCa_{12})(SiO_4)_4\}^{4+}$ and three single AP-layers $\{(FCa_6)(SiO_4)_2\}^{3+}$.

This entire group of minerals is characterized by modular structures containing single $\{[WB_6](TO_4)_2\}$ or triple $\{[W_3B_{12}](TO_4)_4\}$ anti-perovskite layers intercalated with single $A(TO_4)_2$ layers, where A = Ba, K, Sr...; B = Ca, Na...; T = Si, P, V^{5+}, S^{6+}, Al...; W = O^{2-}, F^-. Different combinations of modules along (001) result in different c-parameters (GALUSKIN et al., 2017c). Minerals with structures build by a 1:1 stacking of the single AP-layers and single $A(TO_4)_2$ layer have $c \approx 26$ Å. Triple antiperovskite layers intercalated with single $A(TO_4)_2$ layers result in $c \approx 41$ Å.

The structure of our 'new' mineral, with $c \approx 66$ Å, comprises modules of two other new minerals ariegilatite $BaCa_{12}(SiO_4)_4(PO_4)_2F_2O$ (IMA 216-100), with $c \approx 41$ Å, and stracherite $BaCa_6(SiO_4)_2[(PO_4)(CO_3)]_2F$ (IMA 2016-098), with $c \approx 26$ Å (GALUSKIN et al., 2017a, b).

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