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Fantappièite, a new mineral of the cancrinite-sodalite group with a 33-layer stacking sequence: Occurrence and crystal structure

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Abstract

This paper reports the occurrence and the crystal structure of fantappièite, a new member of the cancrinite-sodalite group of minerals from Torre Stracciacappe, Trevignano community (Rome, Latium, Italy). The mineral occurs within a volcanic ejectum consisting of dominant sanidine with minor plagioclase, biotite, augitic clinopyroxene, andradite, and iron oxides. Fantappièite (0.7 mm as largest size) is observed within miarolitic cavities of the rock as transparent colorless crystals, showing complex morphologies and striated faces. It is non-pleochroic and uniaxial negative, $n_\omega = 1.5046(5)$ and $n_\varepsilon = 1.5027(5)$. D_{calc} is 2.471 g/cm^3. Fantappièite is trigonal, space group $P\bar{3}$; the cell parameters are: $a = 12.8742(6)$, $c = 87.215(3)$ Å, $V = 12518.8(9)$ Å^3, $Z = 1$. The empirical chemical formula is: $(Na_{84.12}Ca_{30.00}K_{15.95}Fe_{0.19}Ti_{0.13}Mn_{0.10}Mg_{0.09})(Si_{99.36}Al_{98.64})O_{396}(SO_4)_{30.24}(CO_3)_{0.29}Cl_{0.84}F_{0.82}\cdot 5.18H_2O$, which corresponds to the ideal formula $[Na_{82.5}Ca_{33}K_{16.5}]_{\Sigma=132}(Si_{99}Al_{99}O_{396})(SO_4)_{33}\cdot 6H_2O$.

The five strongest reflections in the X-ray powder pattern are [*d* in Å (*I*%) (*hkl*)]: 3.70 (100) (3 0 0), 3.60 (80) (1 0 23), 2.641 (65) (0 0 33), 6.85 (60) (0 1 10), 6.40 (55) (1 1 0).

The single-crystal FTIR spectrum rules out OH groups and shows the presence of H_2O and CO_2 molecules, as well.

The structure can be described as a stacking sequence of 33 layers of six-membered rings of tetrahedra along the *c* axis. The stacking sequence is ACBACABACBACBACBCACBACBACBAB-CBACB…, where A, B, and C represent the positions of the rings within the layers. This sequence gives rise to liottite, sodalite, and cancrinite cages, alternating along *c*. Sulfate groups occur within the liottite cages associated by Na, K, and Ca, while highly disordered sulfate groups are located within the sodalite cages. H_2O groups occur within the cancrinite cages, bonded to Ca and Na cations. Split positions are found for Na-Ca sites, and are related to disordering of the sulfate groups in the sodalite cages.

Keywords: New minerals, fantappièite, crystal structure, IR spectroscopy, mechanical properties