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Kircherite, a new mineral of the cancrinite-sodalite group with a 36-layer stacking sequence: Occurrence and crystal structure

Fernando Cámara,[1] Fabio Bellatreccia,[2,*] Giancarlo Della Ventura,[2] Mickey E. Gunter,[3] Marco Sebastiani,[4] and Andrea Cavallo[5]

[1]Dipartimento di Scienze della Terra, Università di Torino, Via Valperga Caluso 35, I-10125 Torino, Italy
[2]Dipartimento di Scienze Geologiche, Università Roma Tre, Largo San Leonardo Murialdo 1, I-00146 Rome, Italy
[3]Department of Geological Sciences, University of Idaho, Moscow, Idaho, 83844-3022, U.S.A.
[4]Dipartimento di Ingegneria Meccanica e Industriale, Università Roma Tre, Via della Vasca Navale 79, I-00146 Rome, Italy
[5]Istituto Nazionale di Geofisica e Vulcanologia (I.N.G.V.), Via di Vigna Murata 605, I-00143 Rome, Italy

Abstract

This paper reports on the occurrence and the crystal structure of kircherite, a new member of the cancrinite-sodalite group of minerals from Valle Biachella, Sacrofano community (Rome, Latium, Italy). The mineral occurs in association with sodalite, biotite, iron oxides, titanite, fluorite, and a pyrochlore-group mineral. The groundmass of the ejectum consists essentially of K-feldspar with subordinate plagioclase. Kircherite (3 mm as largest size) is observed within miarolitic cavities of the rock and typically occurs as parallel associations of hexagonal, thin, tabular colorless to light-gray transparent crystals; it is non-pleochroic and uniaxial negative, with $\omega = 1.510(2)$ and $\varepsilon = 1.502(2)$. D_{calc} is 2.457 g/cm^3. Kircherite is trigonal with $a = 12.8770(7)$, $c = 95.244(6)$ Å, $V = 13677(1)$ Å^3, $Z = 1$. The structure has been refined in the trigonal space group $R32$, obtaining a R-value of 8.5% on 8131 reflections with $I/\sigma I > 2$. The strongest seven reflections in the X-ray powder pattern are [d in Å (I %) (*hkl*)]: 3.717 (100) (3 0 0), 2.648 (100) (2 1 28; 0 0 36), 3.232 (65) (2 1 19), 3.584 (60) (1 2 14), 3.604 (53) (1 0 25), 3.799 (52) (1 2 11), 3.220 (38) (2 2 0). The single-crystal FTIR spectrum rules out OH groups and shows the presence of H_2O and CO_2 molecules in the structural cages of the mineral. Chemical analysis gives (in wt%): SiO_2 32.05, Al_2O_3 27.13, FeO 0.07, K_2O 4.38, CaO 8.75, Na_2O 13.62, MgO 0.01, MnO 0.02, TiO_2 0.01, SO_3 12.87, Cl 0.35, F 0.05, total 99.82. The empirical formula calculated on the basis of $\Sigma(Si+Al) = 216$ apfu is $(Na_{89.09}Ca_{31.63}K_{18.85}Fe_{0.20}Mn_{0.06}Mg_{0.05}Ti_{0.03})_{\Sigma=139.91}[(Si_{108.13}Al_{107.87})_{\Sigma=216.00}O_{430.00}](SO_4)_{32.58}Cl_{2.00}F_{0.53}\cdot 6.86H_2O$, which corresponds to the ideal formula $[Na_{90}Ca_{36}K_{18}]_{\Sigma=144}(Si_{108}Al_{108}O_{432})(SO_4)_{36}\cdot 6H_2O$.

The structure can be described as a stacking sequence of 36 layers of six-membered rings of tetrahedra along the **c** axis. The stacking sequence is ACABCABCABCACBCABCABCABCBABCAB-CABCAB…, where A, B, and C represent the positions of the rings within the layers. This sequence gives rise to cancrinite, sodalite, and losod cages, alternating along **c**. Sulfate groups occur within the sodalite and losod cages associated by Na, K, and Ca. H_2O groups occur within the cancrinite cages, bonded to Ca and Na cations. Anion groups (SO_4^{2-}) in sodalite cages show positional disorder, and so do consequently the extraframework cation sites related to them.

Keywords: New minerals, kircherite, ordered interstratified sodalites-cancrinite, crystal structure, IR spectroscopy, mechanical properties