ACTA UNIVERSITATIS SZEGEDIENSIS

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ACTA
MINERALOGICA-PETROGRAPHICA
ABSTRACT SERIES

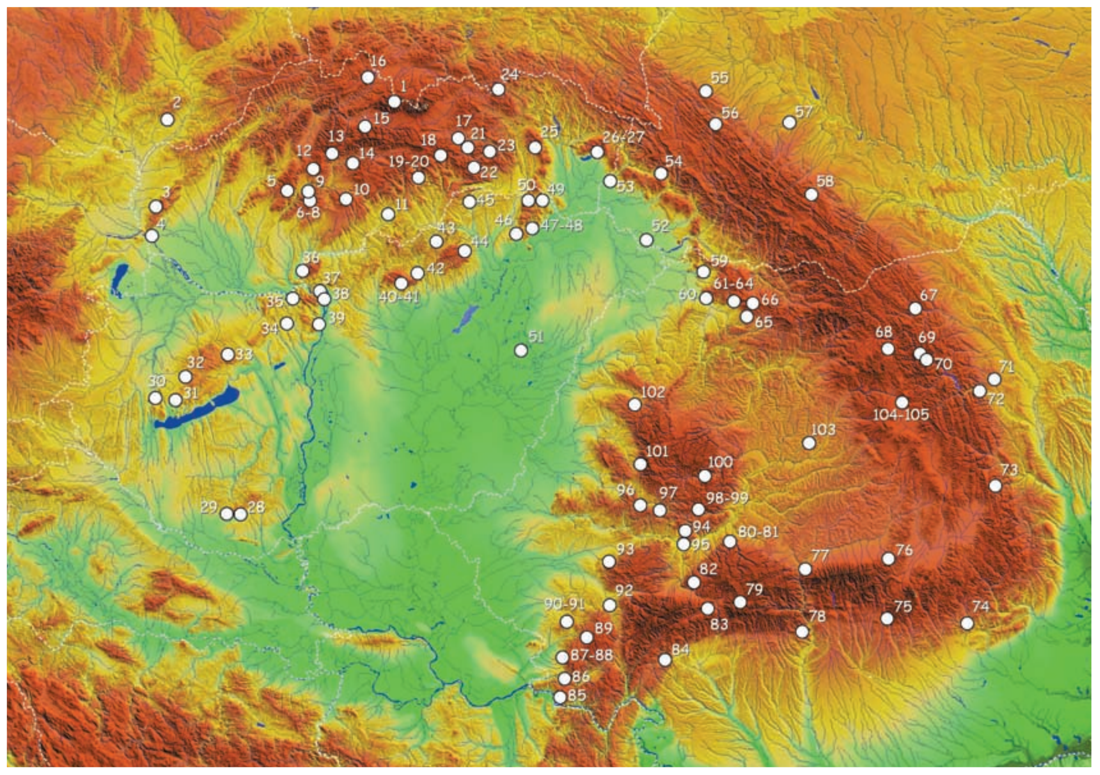
Volume 6 2010

IMA2010

20th General Meeting of the
International Mineralogical Association
21–27 August, 2010

Budapest, Hungary

NKTH
National Office for Research and Technology



Published by the Department of Mineralogy, Geochemistry and Petrology, University of Szeged

Classification and potential new minerals in the "mayenite group"

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The natural analogue of "Cl-mayenite" ($Ca_{12}Al_{14}O_{32}Cl_2$) and "Fe-wadalite" ($Ca_{12}Fe_8Si_6O_{32}Cl_8$), two new potential minerals, were discovered in the altered calcareous silicate xenoliths in ignimbrites of Upper Chegem caldera, Northern Caucasus, Kabardino-Balkaria, Russia. "Cl-mayenite" was formed from mayenite $^{VIII}Ca_{12}(^{IV}Al_8)^1(^{IV}Al_6)^2O_{33}$ by $O^{2-} = 2Cl^-$ replacement, for example $Ca_{12}[Al_{12.98}Fe^{3+}_{0.81}Si_{0.16}Ti^{4+}_{0.04}S^{6+}_{0.01}]_{14.00}O_{31.98}(OH)_{0.05}Cl_{2.28} \times 3H_2O$ [1]. Further, substitutions of Al^{3+} (Fe^{3+}) → $Si^{4+} + Cl^-$, $2Al^{3+}$ (Fe^{3+}) → $Si^{4+} + Mg^{2+}$ and $Ca^{2+} + Al^{3+}$ (Fe^{3+}) → $Na^+ + Si^{4+}$ generated wadalite, $[Ca_{12.01}Na_{0.14}]_{12.15}[Al_{9.21}Si_{4.07}Mg_{0.15}Fe^{3+}_{0.46}Ti^{4+}_{0.03}Mn_{0.02}]_{13,95}Cl_{5.44}F_{0.03}$ and "Fe-wadalite" $[Ca_{12.10}Na_{0.02}]_{12.12}[Fe^{3+}_{9.07}Si^{4+}_{3.2}Al_{1.55}Ti_{0.06}V^{5+}_{0.01}]_{13.88}Cl_{4.91}$.

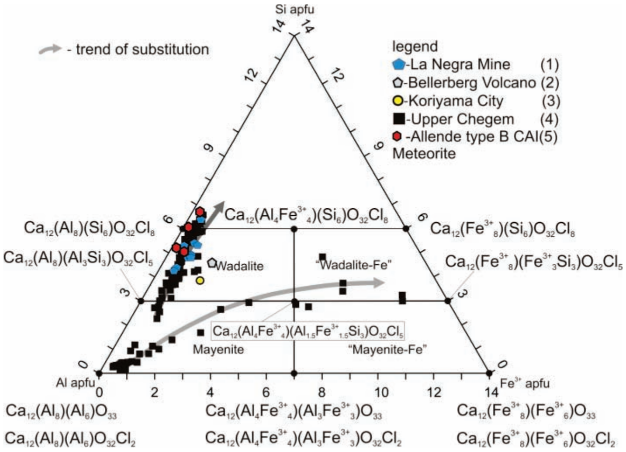

Fig. 1: Classification Si-Al-Fe^{3+}(apfu) diagram of "mayenite group" minerals: (1) wadalite from La Negra mine, Mexico [2]; (2) wadalite from Bellerberg Volcano, Germany [3]; (3) holotype wadalite from Koriyama City, Japan [4]; (4) Minerals of the "mayenite group" from Upper Chegem, Russia; (5) wadalite from Allende type B CAI meteorite [5].

Shorter Al^2-O distances compared with Al^1-O can be related to the prevailing substitution of Si in the Al^2 site [6]. The maximum number of substituted Al atoms by Si in the Al^2 site is 6 apfu [6]. Based on this fact, we propose the boundary between mayenite and wadalite-like minerals at 3 Si pfu. Some wadalite analyses show Si content higher than 6 apfu (Fig. 1), because the small amount of Si goes to the Al^1 site. The Fe^{3+} substitution of Al determines the Fe-rich wadalite and further "Fe-wadalite". The presence of a poorly bonded O atom facilitates its exchange by $2(Cl^-,OH^-)$, giving phases of composition $Ca_{12}Al_{14}O_{32}[O,(OH)_2,Cl_2]$ [7].

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

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We relate here the occurrence and the crystal structure of kircherite (IMA 2009-084), a new member of the cancrinite-sodalite group of minerals from Valle Biachella, Sacrofano, (Rome), in the Sabatini volcanic complex, Latium, Italy. The mineral occurs within miarolitic cavities of holocrystalline, syenitic, volcanic ejecta, associated with sodalite, biotite, iron oxides, titanite, fluorite, and a pyrochlore group mineral. The groundmass of the ejecta consists essentially of potassium-feldspar, with minor sodalite and brown mica.

Kircherite occurs typically as parallel associations of hexagonal, thin, tabular crystals (2 or 3 mm in diameter and 1 mm in thickness). Single platelets have a thickness that very rarely exceeds 0.5 mm. Crystals are colourless to light gray to white, translucent to opaque in the most altered parts of the crystals; lustre is greasy to silky. Fluorescence is in light pink under LW UV and deep red under SW UV. Hardness is (Mohs): 5.5; micro-indentation VHN load 10 g, mean 648.4 kg mm^{-2}, range ± 208.9 kg mm^{-2}. Cleavage on {001} is good. Density (calc.) is 2.457 g cm^{-3}. Kircherite is non-pleochroic and uniaxial negative with $\omega = 1.510(2)$, $\varepsilon = 1.502(2)$.

Kircherite is trigonal, space group *R*32, with , $a = 12.8770(7)$ Å, $c = 95.224(6)$ Å, $V = 13677.2(13)$ Å^3, $Z = 1$. The empirical chemical formula obtained from EMP analyses is: $(Na_{89.09}Ca_{31.63}K_{18.85}Fe_{0.20}Mn_{0.06}Mg_{0.05}Ti_{0.03})_{\Sigma=139.91}(Si_{108.13}Al_{107.87})_{\Sigma=216.00}O_{430.08}(SO_4)_{32.59}Cl_{2.00}F_{0.53}(CO_3)_{0.09}\cdot 6.86H_2O$, 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 strongest six reflections in the X-ray powder pattern are [*d* in Å (I %) (*hkl*)]: 3.72 (100) (300), 2.65 (100) (2.1.28; 0.0.36), 3.23 (65) (2.1.19), 3.58 (60) (1.2.14), 3.60 (53) (1.0.25), 3.80 (52) (1.2.11).

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.

The structure can be described as a stacking sequence of 36 layers of six-membered rings of tetrahedra along the *c* axis as ACABCABCABCACBCABCABCABCBABCABCABCAB…, where A, B and C represent the positions of the rings within the layers. The structure has 6 cancrinite cages (ϵ), 24 sodalite cages (S) and 6 LOSOD cages (L) within the unit cell, and these account for a maximum of 36 SO_4^{2-} groups and 6 H_2O molecules (or Cl anions). There is a unique sequence of cages, ϵSSSLSSLSSSϵ and adjacent sequences are shifted 1/3 along [001]. Kircherite, having 36 layers, is the cancrinite with the longest complex sequence described to date.

The name is for Athanasius Kircher (1602–1680), a German Jesuit who was the founder of the museum of the Collegium Romanum in 1651, hereafter named the Museum Kircherianum.