

s5.m15.p8 **Cation ordering in the new Fe-rich amphibole potassicarfvedsonite.** Yu.S. Lebedeva<sup>1</sup>, D.Yu. Pushcharovsky<sup>1</sup>, I.V. Pekov<sup>1</sup>, G. Ferraris<sup>2</sup>, A.A. Novakova<sup>3</sup> & A. Gula<sup>2</sup>. <sup>1</sup>Faculty of Geology, Moscow State University, Russia. <sup>2</sup>Department of Mineralogy and Petrology, University of Torino, Italy. <sup>3</sup>Faculty of Physics, Moscow State University, Russia. E-mail: yuleb@mail.ru

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The results of the crystal structure investigation and cation ordering obtained by means of X-ray Diffraction analysis and Mössbauer spectroscopy for new monoclinic Fe-rich amphibole potassicarfvedsonite are presented.

Potassicarfvedsonite, ideally  $\text{KNa}_2\text{Fe}^{2+}_4\text{Fe}^{3+}_4\text{Si}_8\text{O}_{22}(\text{OH})_2$ , is a new mineral species of the amphibole group found in alkaline pegmatites in agpaitic complex Ilímaussaq (Greenland). The monoclinic crystal structure with the unit-cell parameters are  $a$  10.002(2),  $b$  18.054(3),  $c$  5.319(1)Å,  $\beta$  103.90(3)°,  $V$  932.4(3)Å<sup>3</sup>, sp. gr.  $C2/m$ ,  $Z=2$ , has been refined by the SHELX97 programs to  $R(F) = 2.29\%$  for 3296 independent reflections with  $I_0 > 2\sigma(I_0)$ . The distribution of the cations over the five independent positions  $M1$ ,  $M2$ ,  $M3$ ,  $M4$  and  $A$  (split into three subsites) was obtained on the basis of X-ray diffraction analysis and Mössbauer spectroscopy. In the  $A$  site a deficiency of cations occurs together with dominant K and minor Na. This site turned out to be split into three subsites: two on the mirror plane ( $A'm$  and  $A''m$ ) and one on the twofold axis ( $A2$ ).

Room temperature Mössbauer spectrum ( $V \pm 4$  mm/s,  $\chi^2$  1.15) was resolved into six quadrupole doublets due to both divalent and trivalent iron in each of the three octahedral positions  $M1$ ,  $M2$ ,  $M3$ , and allowed to estimate  $\text{Fe}^{2+}/\text{Fe}^{3+}$  ratio = 2.61. No signal corresponding to tetrahedral  $\text{Fe}^{3+}$  was detected.

The peculiar structural features of this amphibole are discussed in connection with its genesis.

s5.m15.p9 **Models of the modular structures of two new heterophyllosilicates related to bornemanite and barytolamprophyllite.** P. Németh<sup>a</sup>, G. Ferraris<sup>a</sup>, I. Dódy<sup>b</sup>, G. Radnóczy<sup>c</sup> and A.P. Khomyakov<sup>d</sup>, <sup>a</sup>Dpt. of Mineralogical and Petrologic Sciences, University of Torino, Torino, Italy, <sup>b</sup>Mineralogical Dpt., Eötvös L. University, Budapest, Hungary, <sup>c</sup>Research Institute for Technical Physics and Material Sciences, Budapest, Hungary, <sup>d</sup>IMGRE-RAS, Moscow, Russia. E-mail: peter.nemeth@unito.it

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Titanosilicates are a prominent part of new minerals from Lovozero and Khibiny Massif (Kola Peninsula, Russia) [1]. The number of new species and the interest for them is continuously increasing. About 30 natural layer titanosilicates belong to the bafertisitite polysomatic series and are members of the wider series of the heterophyllosilicates [2]. Their structure is based on a  $HOH$  bafertisitite-like layer where  $H$  (for hetero) is a phyllosilicate-like tetrahedral sheet with inserted rows of five- or six-co-ordinated Ti(Nb), and  $O$  is an octahedral sheet. Ideally, the members of the bafertisitite series have formula  $A_2Y_4[(\text{Ti,Nb})_{2+p}(\text{O})_2\text{Si}_4\text{O}_{14}](\text{O}')_2$  where  $A$  = interlayer cations,  $Y$  = octahedral cations,  $O'$  (bonded to Ti) and  $O''$  (belonging to the  $O$  sheet) are  $O$ ,  $\text{OH}$ ,  $\text{F}$  and  $\text{H}_2\text{O}$ . The value of  $p$  (0,1) depends on the Ti coordination and linkage. Basing on chemical data, selected area electron diffraction (SAED), high resolution electron microscopy images (HRTEM), X-ray powder diffraction data and systematic comparison with parent and other related structures according to the principles of modular crystallography [3], we have obtained appropriate structure models for two new heterophyllosilicates, labelled M72 and M73 in [1]. These two minerals are high-hydrated derivatives of bornemanite and barytolamprophyllite, in the order. M72 derives from bornemanite following the leaching of the phosphate anions and further hydration; besides, a part of Ti changes its coordination from six to five and the seidozerite-like module is transformed into a lamprophyllite-like module. M72,  $\text{BaNa}\{(\text{Na,Ti})_4[(\text{Ti,Nb})_2(\text{OH},\text{O})_2\text{Si}_4\text{O}_{14}](\text{OH},\text{F})_2\} \cdot 3(\text{H}_2\text{O})$ , occurs as two polytypes:  $a = 5.552(1)$ ,  $b = 7.179(1)$ ,  $c = 25.47(1)$  Å,  $\gamma = 91.10(1)^\circ$  ( $P11m$  polytype); same  $a$  and  $b$ , double  $c$  ( $I11m$  polytype). M72, besides the mentioned lamprophyllite-like module, contains a second module which, in the bafertisitite series, is new for its interlayer content. For comparison, the structure of bornemanite,  $\text{BaNa}_3\{(\text{Na,Ti})_4[(\text{Ti,Nb})_2\text{O}_2\text{Si}_4\text{O}_{14}](\text{OH},\text{F})_2\} \text{PO}_4$ , is based on modules of seidozerite,  $\text{Na}_2\{(\text{Na,Mn,Ti})_4[(\text{Zr,Ti})_2\text{O}_2\text{Si}_4\text{O}_{14}]\text{F}_2\}$ , and lomonosovite,  $\text{Na}_8\{(\text{Na,Ti})_4[\text{Ti}_2\text{O}_2\text{Si}_4\text{O}_{14}](\text{O},\text{F})_2\}(\text{PO}_4)_2$ . M73 has composition  $(\text{Ba,Na})_2\{(\text{Na,Ti})_4[(\text{Ti,Nb})_2(\text{OH})_3\text{Si}_4\text{O}_{14}](\text{OH},\text{F})_2\} \cdot 4(\text{H}_2\text{O})$  and derives from barytolamprophyllite,  $(\text{Ba,Na})_2\{(\text{Na,Ti})_4[\text{Ti}_2\text{O}_2\text{Si}_4\text{O}_{14}](\text{OH},\text{F})_2\}$ , by further hydration and differentiation of the interlayer content into two distinct ones. M73 occurs as two polytypes:  $a = 5.40(2)$ ,  $b = 6.88(2)$ ,  $c = 24.01(3)$  Å,  $\beta = 91.3(2)^\circ$  ( $P2/m$  polytype); same  $a$  and  $b$ , double  $c$  ( $A2/m$  polytype).

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