ON THE CRYSTAL STRUCTURE OF ‘BETA-LOMONOSOVITE’

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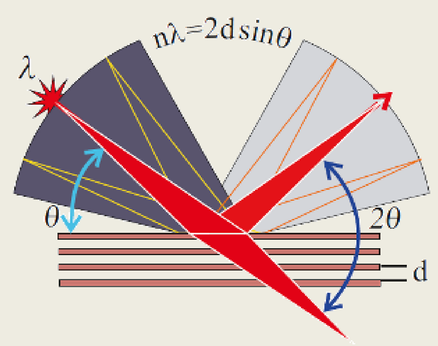

‘Beta-lomonosovite’, $Na_4Ti_4Si_4O_{18}\cdot Na_3[PO_3(OH)PO_2(OH)_2]$, is a titanosilicate from the murmanite - lomonosovite family, which is currently discredited as a mineral species [1]. The purpose of this work is to study the crystal structure of ‘beta-lomonosovite’ in order to establish its possible identity as a separate mineral species. The sample of the mineral originated from the Apatite Circus mineral deposit, Khibiny Massif (Fig.1).

Fig.1. The crystal of ‘beta-lomonosovite’ (1.5 cm), Apatite Circus mineral deposit

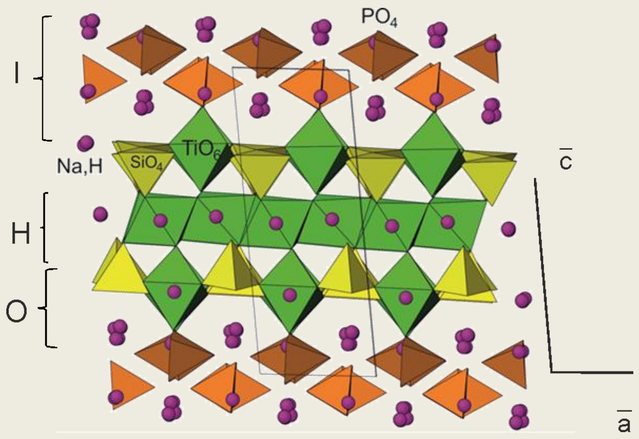

Fig.2. The crystal structure of ‘beta - lomonosovite’. Projection on plane (010)

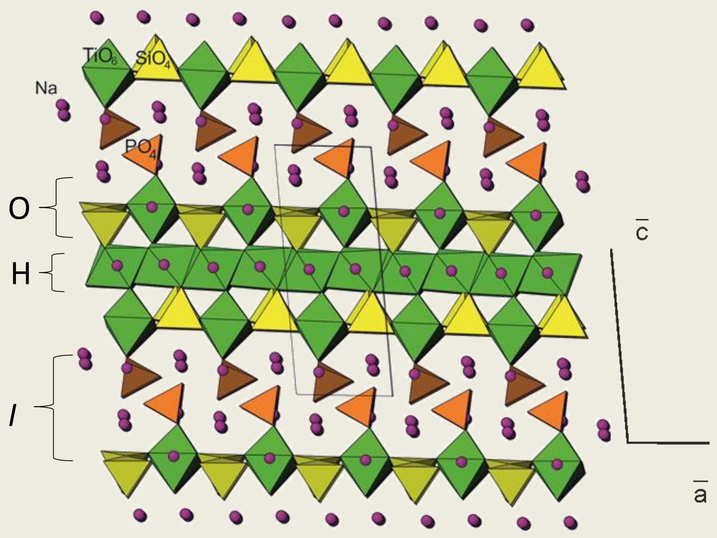

Fig.3. The crystal structure of lomonosovite. Projection on plane (010)

The crystal structure of mineral was studied by single crystal X-ray diffraction analysis by means of the Bruker Smart Apex II diffractometer equipped with the CCD area detector (Fig.2). Beta-lomonosovite is triclinic, *P*-1, a = 5.327(2), b = 14.161(4), c = 14.495(4) Å, α = 102.94(2), β = 96.32(2), γ = 90.28(3)°, V = 1058.8(5) Å^3 . The structure consists of chains of PO_4 tetrahedra and TiO_6 octahedra running parallel to the c axis. The $P1O_4$ tetrahedron occupies a position analogous to that in lomonosovite and the $P2O_4$ is turned towards the opposite side [2].

In agreement with previous reports [3], structure refinement indicated that there are several under-occupied Na sites, which is most probably related to the protonation of some of the PO_4 tetrahedra. Analysis of tetrahedra distortion indicated that each of the two PO_4 tetrahedra has two potential O sites available for protonation. Ordering of the under-occupied Na sites and distortions of the PO_4 tetrahedra result in doubling of the unit cell compared to that in lomonosovite (Fig.4).

The chemical composition (wt. %) of ‘beta - lomonosovite’ (Si+Al = 4)

Na	6.93 – 8.15
K	0.00 – 0.02
Ca	0.23 – 0.26
Mn	1. – 0.05
Mg	0.00 - 0.03
Fe	0.18 – 0.20
Ti	3.73 – 3.89
Nb	0.06 – 0.19
Al	0.00 – 0.01
Si	3.99 – 4.00
P	1.99 – 2.02
F	0.00 – 0.22

Selected Bond Lengths [Å] in the PO_4 tetrahedra

P1-O17	1.500(3)
P1-O22	1.505(4)
P1-O21	1.530(5)
P1-O19	1.533(5)
<P1-O>	1.517
P2-O23	1.494(5)
P2-O16	1.497(4)
P2-O24	1.515(4)
P2-O20	1.544(6)
<P2-O>	1.51
P2A-O23	1.371(6)
P2A-O16	1.449(5)
P2A-O20A	1.52(2)
P2A-O24	1.564(6)
<P2A-O>	1.48

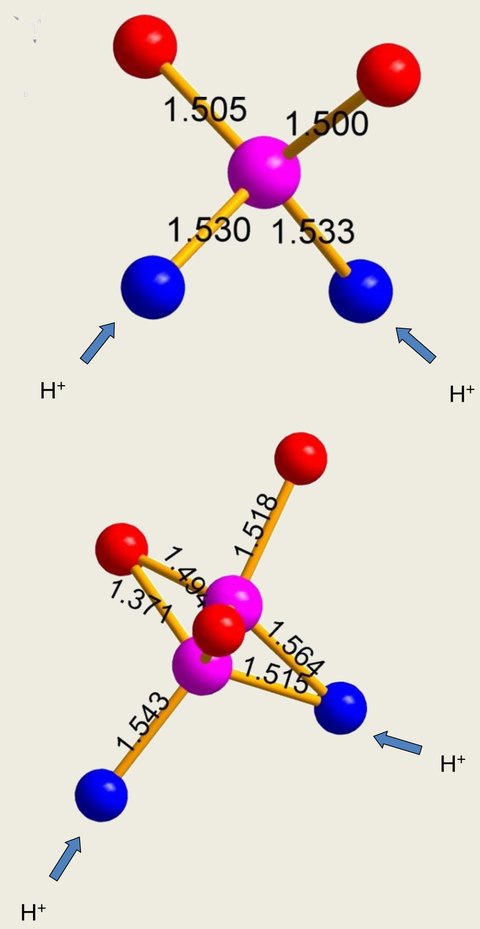

Fig.4. The PO_4 tetrahedra in the structure of ‘beta - lomonosovite’

According to the structural refinement and chemical-analysis data the crystal chemical formula was calculated $Na_{7.4}Ca_{0.24}Fe_{0.09}Mn_{0.02})_{\sum 7.75}(Ti_{3.80}Nb_{0.10}Fe_{0.10})_{\sum 4}(Si_2O_7)_2O_4(HPO_4)_2$.

In conclusion, our studies confirmed previous results and allowed to obtain precise structural information that can be used to investigate status of ‘beta - lomonosovite’ either as a new mineral species or a variety of lomonosovite.

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