Poster

Eveslogite – a highly complex nanotubular titanosilicate mineral solved by 3D ED

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Naturally occurring minerals provide examples of unique nanoscopic tubular units based upon silicate oxyanions. The crystal structure of eveslogite (first described in [1]), a chemically and structurally complex natural Ca-K-Ba-Ti-Fe-Nb silicate from the Eveslogchorr Mt., Khibiny massif, located in the Russian Arctic, solved using 3D electron diffraction (3D ED) provides an amazing example of binary nanotubular structure formed by two type of tubules, one of which is an analogue of the yuksporite [2] nanorod with elliptical cross-section, whereas the other is new and represent a Nb-modified variety of the charoite [3] tubule.

Most datasets came from twinned crystals, but a few corresponded to untwinned crystals. The unit cell refined against the powder diffraction data differed only slightly from the 3D ED cell, namely a = 14.2358(2) Å, b = 44.8239(5) Å, c = 15.9058(4) Å, β = 109.658(2). Figure 1 shows the resulting crystal structure of eveslogite in projection along ***a*** axis. The unit cell contains 345 independent atom positions. The skeleton of the structure consists of 62 SiO_4 tetrahedra, which form chains and two different kinds of tubules that run parallel to [100]. Adjacent to the tubules, there are 13 polyhedra. Four of them contain highly scattering species, which were attributed to a mixed-occupancy Ba/Sr sites and the remaining nine were interpreted as K atoms. Seven K atoms at 0.5 occupancy were located in the interior of the tubules. Two octahedra of one tubule are occupied by Ti/Nb. The other tubule contains eight $(Ti,Nb,Fe,Mn)O_6$ octahedra. The ratio of cations in these positions was set and fixed to the values corresponding to the average chemical composition estimated by EDS, leading to an occupancy for each M position of 0.740, 0.048, 0.134 and 0.079 for Ti, Nb, Fe and Mn, respectively. The same procedure was followed with the $(Fe,Mn)O_5$ square pyramid, where the occupancies were set to 0.63 and 0.37 for Fe and Mn, respectively. The tubules are inter-connected by forty independent (Ca,Na)Ox polyhedra that form ribbons parallel to [100].

The topological analysis of interpolyhedral connectivity shows that the walls of the nanotubules possess topologies of lamprophyllite and delhayelite-group minerals and most probably were formed through the natural exfoliation processes well-known in current 'soft- chemistry' nanotechnology. The information-based structural complexity calculations indicate that eveslogite is the seventh most complex mineral known so far.

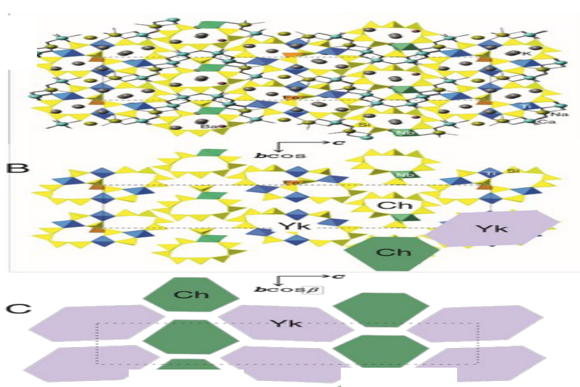

Figure 1. The crystal structure of eveslogite - projection of the full crystal structure along ***a*** axis.

[1] Menshikov Yu.P. et al. (2003). *Obshch.*, **132**, 59 (in Russian, English abs.).

[2] Krivovichev S.V. et al. (2004). *Amer. Miner.*, **89**, 1561.

[3] Rozhdestvenskaya, I. V. et al. (2017). *IUCrJ*, **4**, 223.

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