Eveslogite – Decoding the complexity of eveslogite through three-dimensional electron diffraction

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Eveslogite is an exceptionally complex mineral, found exclusively at Mt. Eveslogchorr, located in the Khibiny alkaline massif, Kola peninsula, Russia. It occurs as a late-hydrothermal formation in veins breaching a poikilitic nepheline syenite, called rischorrite. Despite its discovery in 2003, the structure of eveslogite remained elusive due to its intricacies and the limitations of available methods and instruments at that time (Men'shikov et al. 2003). It was originally thought that the structure resembled that of a heterophyllosilicate (Ferraris & Gula, 2005), but doubts regarding the applicability of the modular approach arose after the crystal structure of a similar mineral, yuksporite, was determined (Krivovichev et al., 2004). To overcome these challenges, advanced techniques such as three-dimensional electron diffraction (3DED; Gemmi et al., 2019) was used to determine the structure and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) was employed to verify it. These methods allowed the investigation of the eveslogite structure at the nanoscale, as the small crystal size and complex twinning prevented the use of traditional X-ray diffraction techniques. Additionally, energy dispersive X-ray spectroscopy (EDS) provided valuable insights into the elemental composition of the mineral. Contradictory previous findings (Men'shikov et al., 2003) new cell parameters were proposed (a = 14.2359 Å, b = 44.8242 Å, c = 15.9058 Å, α = 90°, β = 109.658°, γ = 90°, with a cell volume of 9558.08 Å^3) and the space group $P2_1$ was unambiguously assigned. This revised cell facilitated the structure determination of eveslogite, which comprises 345 symmetrically independent atom positions [see Figure 1(A)]. Based on the average elemental composition the sum formula of eveslogite is $K_{17.5}(Ba,Sr)_8(Na,Ca)_{40}[(Ti,Nb,Fe,Mn)_{11}Si_{62}O_{179}(OH,F)_{12}(O,OH)_{13}](H_2O)$. The essential building blocks that make up the eveslogite structure are heterosilicate tubular chains (see Figure 1(B) and (C)) as well as double-tubes (see Figure 1(D) and (E)), extending along the a-axis. Zig-zag rows of the tubular building units are interconnected by ribbons of $(Ca,Na)O_x$ polyhedra likewise extending along [100]. The heterosilicate tubular building units of eveslogite show a certain degree of similarity with silicate-only modules occurring in charoite and denisovite (Rozhdestvenskaya et al., 2010; Rozhdestvenskaya et al., 2017). Additional diortho-silicate groups are always connected with the heteroatoms. The double-tubes consist of unbranched dreier double silicate chains connected via (Ti,Nb,Fe,Mn)-heterocations (M) to diortho-silicate groups, resembling the structure of yuksporite. Notably, the M positions form MO_6 octahedra or MO_5 square pyramids within the double-tubes. The findings of this research shed light on the complex structure of eveslogite, emphasizing the importance of avoiding twinning and acquiring data from single nm-sized crystals using 3DED. This study not only contributes to a deeper understanding of this remarkable mineral but also showcases the power of advanced electron microscopy techniques in unravelling the intricate structures of minerals.

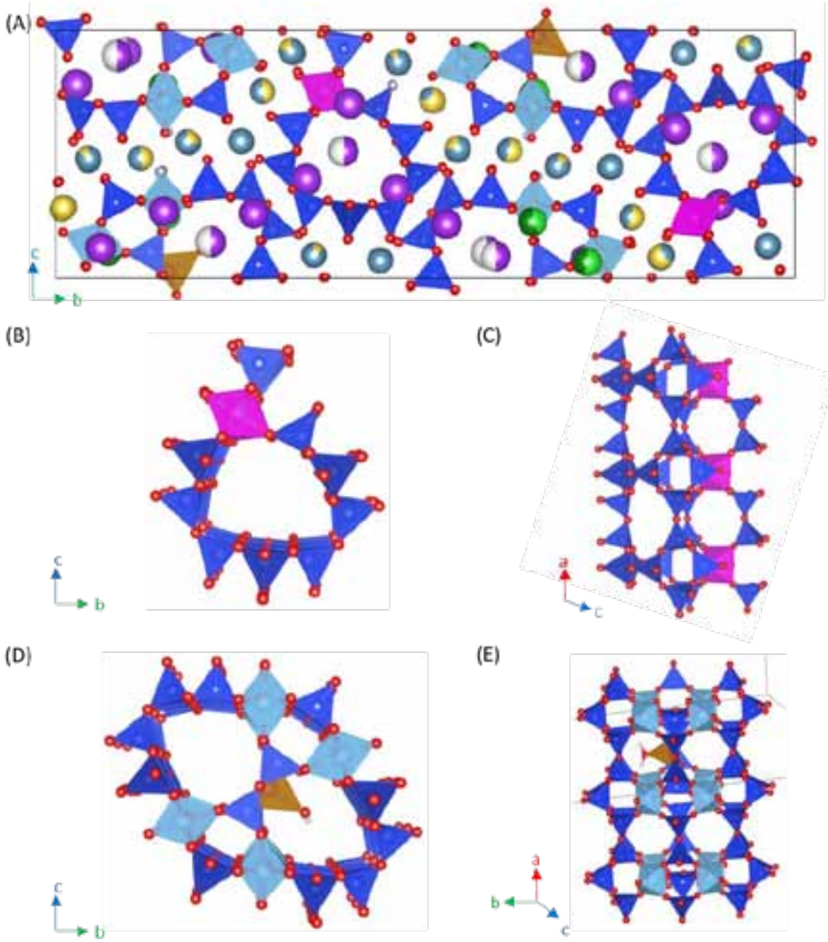

Figure 1: (A) Structure of eveslogite along [100]. The unit cell is marked by a black box. The heterosilicate tubular chains are shown along [100] in (B) and along the [010] in (C). (D) and (E) show the double-tube along [100] and along [329], respectively. Si is displayed in dark blue, M in light blue, (Ti,Nb) in pink, (Fe,Mn) in orange, Ba in light green, Sr in dark green, K in purple, Ca in blue-grey, Na in yellow, O in red, F in grey and H in white

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