

s11.m1.p9 Crystal growth and structure of a new yttrium titanate, $Y_{5+x}Ti_{2+y}O_{12}$, related to rutile. U. Kolitsch, *Institut für Mineralogie und Kristallographie, Geozentrum, Universität Wien, A-1090 Wien, Austria, uwe.kolitsch@univie.ac.at*

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Flux growth experiments were run to investigate phase relations in the systems RE_2O_3 - TiO_2 - SiO_2 ($RE = Nd, Gd, Y, Sc$), which contain phases related to trimoussite-(Y) [$(Y,RE)_2Ti_2SiO_9$] and the RE -(Mg,Fe)-titanosilicates perrierite/chevkinite. Crystals of the new yttrium titanate $Y_{5+x}Ti_{2+y}O_{12}$ (with $x = 0-0.33$ or $y = 0-0.25$) were grown from a LiF-MoO₃ flux at 1050 - 850°C in air. The crystal structure (space group $C2/m$, $a = 12.226(2)$, $b = 5.885(1)$, $c = 7.135(1)$ Å, $\beta = 106.99(3)^\circ$, $Z = 8$) was determined using single-crystal diffractometer data (CCD area detector, MoK α X-radiation) and refined to $R = 2.24\%$.

The structure contains three Y-O polyhedra and infinite chains of edge-sharing TiO_6 octahedra along the b -axis (with alternating short and long Ti-Ti distances, 2.839 and 3.046 Å). Apical O atoms of the $Y(3)O_6$ octahedra link the TiO_6 chains within the (100) plane. Sheets of YO_7 polyhedra parallel to (100) link the chains along the a -axis. $Y_{5+x}Ti_{2+y}O_{12}$ shows the basic topology of $Y_5Mo^{4.5+}_2O_{12}$ and $RE_5Re^{4.5+}_2O_{12}$ compounds^{1,2}. However, it contains an additional, octahedrally coordinated and partially occupied cation site at (0,0,0.5), which is needed for charge compensation. This site is probably occupied by a mixture of major Y and minor Ti, and was designated Y(4). The suggested general formula is $Y_{5+x}Ti_{2+y}O_{12}$, with possible end-member compositions $Y_{5.33}Ti_2O_{12}$ ($Y_8Ti_3O_{18}$) and $Y_5Ti_{2.25}O_{12}$ ($Y_{20}Ti_9O_{48}$). If the partially occupied Y(4) site is also taken into account for the structure description, one recognises chains of edge-sharing $Y(3)O_6$ and $Y(4)O_6$ octahedra. These chains also run parallel to the b -axis, and share all their apical O atoms with the parallel TiO_6 chains above and below them. The TiO_6 - $Y(3)O_6$ - $Y(4)O_6$ slab of chains bears strong resemblance to a single (110) slab in the structure of rutile (TiO_2). Similar rutile-type (110) slabs are also known to occur in a series of novel layered titanosilicates, $La_4Ti(Si_2O_7)_2(TiO_2)_{4m}$ ($m = 1,2$). A comparison with the related Mo- and Re-compounds is made, and twinning features of the common structure type are discussed.

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s11.m1.p10 A new, lintsite-related titanosilicate mineral from Russia: crystal structure, occurrence and properties. U. Kolitsch¹, D.Yu. Pushcharovky², I.V. Pekov³, E. Tillmanns¹, ¹*Inst. für Mineralogie und Kristallographie, Geozentrum, Univ. Wien, A-1090 Wien, Austria, uwe.kolitsch@univie.ac.at*, ²*Lomonosov Moscow State Univ., Dept. of Geology, Moscow 119899, Russia, dmitp@geol.msu.ru*, ³*Lomonosov Moscow State Univ., Dept. of Mineralogy, Moscow 119899, Russia*

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The new mineral, which is closely related to lintsite ($Na_3LiTi_5Si_4O_{14} \cdot 2H_2O$), was found at Malyi Punkaruaiv Mountain, Lovozero alkaline massif, Kola Peninsula, Russia. It occurs in a hydrothermally altered hyperalkaline pegmatite. Electron microprobe analyses show only Ti and Si (Ti:Si ratio close to 0.5) and very low Na contents (0.2-0.3, rarely up to 1 wt.% Na₂O); the Li content has not been determined yet. The IR spectrum is clearly different from spectra of the related minerals lintsite, vinogradovite [$(Na,Ca,K)_4Ti_4AlSi_6O_{23}(OH) \cdot 2H_2O$], kukisvumite [$Na_6ZnTi_4Si_8O_{28} \cdot 4H_2O$] and lorenzenite [$Na_2Ti_2Si_2O_9$]. The mineral forms colourless, elongate {001} tabular {100} crystals up to 1.5 x 0.2 mm, intergrown as bundles and chaotic aggregates in small cavities. It is transparent, with strong pearly lustre, and shows a perfect cleavage // to {100} and a very good cleavage // to {010}.

Single-crystal studies give a monoclinic cell ($C2/c$, $a = 26.68$, $b = 8.77$, $c = 5.22$ Å, $\beta = 91.2^\circ$), similar to that of lintsite ($C2/c$, $a = 28.58$, $b = 8.60$, $c = 5.22$ Å, $\beta = 91.0^\circ$), but with a distinctly smaller a parameter. A structure determination of a crystal fragment of mediocre quality showed the mineral to contain basically the same polyhedral titanosilicate slabs found in lintsite ($R \sim 10\%$ - a triclinic refinement resulted in the same model; twinning was not evident). The slabs consist of chains of edge-sharing TiO_6 octahedra extended along [010], which are connected to pyroxene-like chains of SiO_4 tetrahedra via shared O ligands. These slabs are oriented // to {100} and separated by a widely open space which contains a somewhat disordered and partially occupied, [4]-coordinated Li ion. Its position is identical to the Li position in lintsite. Two O atoms shared by the LiO_4 and $Si(2)O_4$ tetrahedra are disordered, too. There is also evidence that the Si(2) position is only partially occupied. Very small residual electron densities are found close to disordered atoms and the Ow and Na(2) positions of lintsite. The wide spacing between the titanosilicate slabs explains the excellent cleavage // to {100}. The spacing is smaller in the new mineral than in lintsite because there are no two 'space-consuming' Na sites as in lintsite. The relation to the structures of lintsite and vinogradovite will be discussed.

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