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Heftetjernite, a new scandium mineral from the Heftetjern pegmatite, Tørdal, Norway

Uwe KOLITSCH[1,*], Roy KRISTIANSEN[2], Gunnar RAADE[3] and Ekkehart TILLMANNS[4]

[1] Mineralogisch-Petrographische Abt., Naturhistorisches Museum, Burgring, 7, 1010 Wien, Austria
*Corresponding author, e-mail: uwe.kolitsch@nhm-wien.ac.at
[2] PO Box 32, 1650 Sellebakk, Norway
[3] Naturhistorisk Museum, Universitetet i Oslo, Postboks 1172 Blindern, 0318 Oslo, Norway and Norsk Bergverksmuseum, Postboks 18, 3602 Kongsberg, Norway
[4] Institut für Mineralogie und Kristallographie, Geozentrum, Universität Wien, Althanstr. 14, 1090 Wien, Austria

Abstract: Heftetjernite, ideally $ScTaO_4$, is a new scandium mineral from the Heftetjern pegmatite, Tørdal, Telemark, Norway. In the type specimen, it occurs as minute, elongate tabular, very dark brown crystals in a single small void in albite. Other associated minerals are fluorite, muscovite, altered milarite, a metamict, dark greyish brown mineral of the pyrochlore-microlite group, and an unidentified, orange-brown, tabular, nearly X-ray amorphous Ti-Y-Ta-Nb-mineral. Electron-microprobe analysis yielded the empirical formula $(Sc_{0.64}Sn_{0.13}Mn_{0.12}Fe_{0.08}Ti_{0.06})_{\Sigma 1.03}(Ta_{0.69}Nb_{0.30})_{\Sigma 0.99}O_4$ which clearly demonstrates the charge-balanced substitution scheme $2Sc^{3+} = (Sn,Ti)^{4+} + (Mn,Fe)^{2+}$. The mineral crystallises in the wolframite structure type, with space group $P2/c$ and $a = 4.784(1)$, $b = 5.693(1)$, $c = 5.120(1)$ Å, $\beta = 91.15(3)°$, $V = 139.42(5)$ Å^3 ($Z = 2$). A synthetic equivalent is known. Strongest lines in the calculated X-ray powder diffraction pattern of heftetjernite are [d in Å (I) (hkl)]: 3.000 (100) (11–1), 2.9570 (97) (111), 3.662 (53) (110), 2.4877 (34) (02–1), 4.783 (33) (100), 3.807 (32) (01–1). The crystal structure was refined to $R(F) = 1.39$ % from single-crystal X-ray diffraction data (293 K). It is based on two types of edge-sharing, distorted octahedra occupied predominantly by Sc and Ta, respectively.

Heftetjernite is translucent to transparent, with a dark brownish (with a reddish hue) streak and adamantine lustre. It is brittle, has a perfect {010} cleavage, irregular fracture and a Mohs hardness estimated to be around 4.5 by comparison to ferberite; $D_x = 6.44$ g/cm^3 (from crystal-structure analysis). Optically, the mineral is biaxial with an unknown optical sign, weakly pleochroic (yellowish brown with a reddish tint to reddish brown), with no observable dispersion. A mean refractive index of 2.23 was calculated from the Gladstone-Dale relationship using the X-ray density.

Heftetjernite is named after its type locality. The mineral is compared with synthetic $ScTaO_4$, $ScNbO_4$, iwashiroite-(Y) and formanite-(Y) (both nominally $YTaO_4$), and some comments are made on the relation to Sc-bearing ixiolite.

Key-words: heftetjernite, new mineral, scandium tantalate, crystal structure, chemical analysis.

1. Introduction

The year 2003 marked the centennial of the first discovery of a true scandium mineral in nature, *viz.* thortveitite ($Sc_2Si_2O_7$), found in Evje-Iveland in Norway. This centennial was marked by the International Symposium on the Mineralogy and Geochemistry of Scandium in August 2003 in Oslo, organized by the Natural History Museum, University of Oslo. Up to 2003, only nine scandium minerals were described as such. However, in the last 20 years there has been an increasing interest world-wide in scandium minerals and their formation, as well as in the utilisation of scandium in fields of technical application (*e.g.*, scandium alloys, Sc-based doped luminescent materials).

Recent investigation of the Sc-rich Heftetjern granite pegmatite in Tørdal, Telemark, southern Norway, has disclosed a unique assemblage of scandium minerals, like caesian bazzite (Juve & Bergstøl, 1990), scandiobabingtonite, cascandite (Raade & Erambert, 1999) and thortveitite (Kristiansen, 2003), as well as the two new species kristiansenite (Raade *et al.*, 2002) and oftedalite (Kristiansen, 2005; Cooper *et al.*, 2006), some of them observed in intimate coexistence (Raade *et al.*, 2004). In the past five years the total number of mineral species in the Heftetjern pegmatite has increased considerably due to extensive research activity, and today counts *ca.* 60 species. Among them are eleven different Be minerals, a large quantity of minerals containing Ta, Nb, Y, REE, Sn and Ti, and a total of 15 minerals containing Sc in excess of 1 % Sc_2O_3, including rare scandian varieties of helvite and titanite (Raade *et al.*, 2002; Raade & Kristiansen, 2003; Kristiansen, 2009). Although a relatively large number of

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Sc minerals also occur in the miarolitic granite of Baveno, Italy (Gramaccioli *et al.*, 2004, and references therein), the Heftetjern locality is unique because it is a single, relatively small pegmatite and because of its very high number of Sc- and Sc-bearing species (*cf.* Kristiansen, 2009).

The occurrence of scandium minerals in the Heftetjern pegmatite was first recognised by Bergstøl & Juve (1988), who report scandian ixiolite, caesian bazzite, ''scandium microlite'' (unapproved name, see Jambor & Puziewicz, 1990) and other scandian members of the pyrochlore group. One of their scandian ixiolites has 18.80 wt% Sc_2O_3 and a dominance of Sc among the cations, which would make this a new mineral species, as pointed out subsequently (Raade & Kristiansen, 2000a and b; Raade *et al.*, 2002) and to be discussed further below.

In 2004, one of the authors (RK) found a small sample of albite which contained minute elongate transparent dark brown crystals. These crystals subsequently turned out to be a new monoclinic mineral, structurally identical to synthetic $ScTaO_4$, but with minor substitutions of Nb, Sn, Fe, Mn and Ti. The mineral was named heftetjernite, after its type locality. As an aid in pronunciation, the locality name consists of two parts, Hefte and tjern, the latter meaning a small lake (tarn). The new mineral and mineral name were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (no. 2006–056). The holotype specimen is deposited in the Department of Geology, Natural History Museum, University of Oslo, Norway, under catalogue no. 41726 (original sample designation ''RK99/04''). Two further small specimens were found after the mineral had been approved.

2. Geology and geochemistry of the Tørdal pegmatites

The numerous granite pegmatites of the Tørdal area in Telemark are situated within the Nissedal volcano-sedimentary outlier. Both the outlier (1300–1200 Ma) and the older basement (1520–1500 Ma) are intruded by the Tørdal granite (960–850 Ma), which is regarded as the source of the pegmatite swarms (Bergstøl & Juve, 1988). Rb-Sr dating of lepidolite and microcline from the Skarsfjell pegmatite gave ages between 950 and 880 Ma (Neumann, 1960). From trace-element analyses of different rock types, it has been suggested that some of the Sn and a major part of Sc in the amazonite-cleavelandite pegmatites of the area probably have their source in the volcanogenic rocks of the Nissedal outlier, which were penetrated by the pegmatitic fluids (Bergstøl & Juve, 1988).

The Tørdal area is geochemically different from the other granite pegmatite areas in south Norway, being characterised by elevated concentrations of Sn, Sc, Be and Li. Amazonite-cleavelandite pegmatites in Høydalen and at Skarsfjell were described by Oftedal (1942). Here, Li occurs in lepidolite and zinnwaldite, and Sn in cassiterite. Additional findings in these pegmatites are reported by Bergstøl *et al.* (1977), Raade *et al.* (1993) and Kristiansen (1998), including such rare minerals as tveitite-(Y), kuliokite-(Y) and kamphaugite-(Y). Already in 1940s, Oftedal (1943) found that the brown Li-rich micas from Skarsfjell showed a higher Sc content than the micas from thortveitite-bearing dykes in Iveland, Setesdal.

The Heftetjern and Høydalen pegmatites are situated less than 1 km apart, but at different altitudes (~650 and ~450 m asl, respectively) and yet there are major differences in their geochemistry, with the former showing a remarkably strong concentration of scandium and the latter being enriched in Li and F, elements that are typically concentrated in fluids derived from granitic magmas.

The Tørdal pegmatite area can generally be classified as a Li-Sc-Sn province. Oftedal (1956) has discussed the behaviour of certain elements during the replacement of an amazonite paragenesis by a cleavelandite paragenesis in the Tørdal area. Following Černý (1992), the Tørdal pegmatites belong to a mixed LCT-NYF family.

The Heftetjern cleavelandite-amazonite pegmatite is situated in a marshy area between Høydalen and Skarsfjell in Tørdal, Drangedal, Telemark, Norway, at an altitude of ~650 m asl (latitude 8° 45′ 00″ E, longitude 59° 11′ 00″ N). The pegmatites in this area were first explored by some small blastings performed by the previous landowner, John P. Tveit (1909–1978) in the early 1970s. These blastings were aimed at good-quality amazonite, which he had quarried since the early 1940s in his amazonite-lepidolite pegmatite in the nearby Høydalen quarries (Oftedal, 1942; Kristiansen, 1998). Even after the blastings at Heftetjern in fall 1998 and summer 2003, the exposed pegmatite working is still small, being approximately 1 m deep, 2–3 m wide and 10–12 m in length. However, the total length of the steeply dipping pegmatite may be as much as 300 m with a thickness of 5–40 m; the pegmatite strikes NNW-SSE and is partly covered by glacial drift and vegetation (Bergstøl & Juve, 1988).

3. Description and physical properties

The type specimen, ~2 × 2.5 cm, consists mainly of albite with minor violet fluorite, muscovite, traces of altered milarite and a metamict, dark greyish brown mineral of the pyrochlore-microlite group, beside an unidentified, orange-brown, tabular, nearly X-ray amorphous Ti-Y-Ta-Nb-mineral. Heftetjernite occurs in a single small vug in the albite, and appears on the surface or in between the Ti-Y-Ta-Nb-mineral as only a few elongate tabular to columnar, subparallel crystals (max. length *ca.* 0.4 mm, max. width *ca.* 0.1 mm), broken up by cracks (Fig. 1). The tabular form is {100}; no other distinct forms are observable (indistinct outline of crystals), but {010} or {001} are possibly present. No macroscopic twinning was observed. The very small amount of material available for the characterisation precluded measurements of some physical properties.

Heftetjernite is very dark brown (to greenish brown in part) and translucent to transparent with an adamantine lustre. It is

Fig. 1. SEM micrograph (BSE mode) of aggregates of subparallel, tabular crystals of heftetjernite grown on an unidentified, tabular, nearly X-ray amorphous Ti-Y-Ta/Nb-mineral.

non-fluorescent, brittle, with a perfect {010} cleavage and irregular fracture, and a dark brownish (with a reddish hue) streak. The Mohs hardness could not be determined due to lack and size of material, but is estimated to be similar to that of ferberite, about 4.5. The very sparse material and high density value did not allow a direct measurement of the density. The calculated X-ray density is 6.44 g/cm^3 for the fragment used for the crystal-structure solution.

Optically, the mineral is biaxial. The optical character and 2V could not be determined due to the very dark colour of the mineral. Interference colours, observed on tiny fragments, appear more or less normal (not anomalous); hence, dispersion should be weak if present at all. Indistinctly lath-shaped fragments lying on their platy {100} face show weak pleochroism: yellowish brown with a reddish tint perpendicular to the morphological elongation and reddish brown (with stronger absorption) parallel to the morphological elongation. Edge-on fragments show no pleochroism. The optical orientation is unknown. The mean refractive index is 2.23, calculated from the Gladstone-Dale relationship using the X-ray density.

4. Chemical data

Electron-microprobe analyses (EMPA), using a Cameca SX100 instrument, were made on a carbon-coated polished section of two irregular grains measuring approximately 15 × 30 and 15 × 50 μm (measurements conditions: 15 kV, 15 nA, spot size 2 μm). A wavelength-dispersive scan indicated the absence of any other elements with atomic number greater than 8, except those reported here. A total of eight point analyses showed only small variations of the chemical composition (Table 1) and gave the following empirical formula (based on 4 O atoms): $(Sc_{0.64}Sn_{0.13}Mn_{0.12}Fe_{0.08}Ti_{0.06})_{\Sigma 1.03}(Ta_{0.69}Nb_{0.30})_{\Sigma 0.99}O_4$. The simplified formula is (Sc,Sn,Mn,Fe,Ti)(Ta,Nb)O_4 and the ideal formula $ScTaO_4$. The empirical formula provides unambiguous evidence for the charge-balanced substitution scheme $2Sc^{3+} = (Sn,Ti)^{4+} + (Mn,Fe)^{2+}$. We point out that Ti (0.06 apfu) has been grouped together with Sc because Mn + Fe (0.20 apfu) almost exactly matches Ti + Sn (0.19 apfu) and because the overall ABO_4 stoichiometry and charge-balance are well obeyed. Although it is true that Ti in most cases (complex oxide minerals) couples with Nb and Ta, this is not the case for Sc minerals such as heftetjernite. In minerals, Sc is typically substituting for Fe^{3+}, Al^{3+} and $HREE^{3+}$, but it can also replace Ti^{4+}, Sn^{4+}, Zr^{4+} and W^{6+}. In the synthetic pseudobrookite-type oxide compound Sc_2TiO_5 (Kolitsch & Tillmanns, 2003), Sc

Table 1. Results of electron-microprobe analyses of heftetjernite.

Constituent	Wt%	Range	Probe standard
Sc_2O_3	15.59	14.75–16.34	Sc_2O_3
SnO_2	6.93	6.54–7.41	SnO_2
TiO_2	1.61	1.25–2.16	Pyrophanite
MnO	3.02	2.73–3.30	Pyrophanite
FeO	2.07	1.77–2.30	Fe metal
Ta_2O_5	53.58	50.95–55.45	Ta metal
Nb_2O_5	14.25	12.97–15.64	Nb metal
Total	97.05[a]	96.42–98.12	

[a] The relatively low total is caused by instability of the epoxy directly surrounding the embedded grains, which gives a low conductivity.

and Ti atoms are partially disordered in the two octahedrally coordinated metal sites. The literature contains further examples of metal-Sc-Ti-oxides with mixed (Sc,Ti) sites.

The two other known heftetjernite specimens, found after the species had been approved, were analyzed by standardless SEM-EDS, and both were found to have a chemical composition very similar to that of the type material. The first additional specimen, found in 2007, consists of one almost complete, tabular, very dark brown crystal embedded in biotite, associated with K-feldspar and traces of altered milarite. The crystal has the simplified formula$(Sc_{0.61}Mn_{0.13}Sn_{0.12}Fe_{0.10}Ti_{0.06})_{\Sigma 1.02}(Ta_{0.72}Nb_{0.28})_{\Sigma 1.00}O_4$ (average of two spots). The second additional specimen, found in 2008, contains elongate tabular, subparallel, shiny, dark brown crystals (<0.5 mm in length), broken up by cracks in the same way as the type specimen. The crystals are grown on the surface of a metamict platy mineral with a polycrase-like composition and an approximate formula $[U_{0.39}(Y,REE)_{0.31}Fe_{0.17}Ca_{0.13}Mn_{0.11}Pb_{0.07}]_{\Sigma 1.12}(Ti_{1.26}Ta_{0.39}Nb_{0.25})_{\Sigma 1.90}O_6$. Analyses of the heftetjernite gave the simplified formula $(Sc_{0.69}Sn_{0.11}Mn_{0.11}Fe_{0.10}Ti_{0.02})_{\Sigma 1.03}(Ta_{0.77}Nb_{0.29})_{\Sigma 1.06}O_4$. These new analyses confirm the grouping of Ti with Sc in heftetjernite.

The Gladstone-Dale compatibility index was not calculated because neither density nor refractive indices could be determined experimentally.

5. Crystal structure and X-ray powder diffraction data

The crystal structure of heftetjernite was solved from single-crystal X-ray diffraction data collected from a tiny fragment (see Table 2 for details). SHELXS-97 (Sheldrick, 1997a) and SHELXL-97 (Sheldrick, 1997b) were used for solution and refinement of the structure, respectively. Since the structure determination showed that heftetjernite has a wolframite-type structure, the atomic coordinates of hübnerite, $MnWO_4$ (Weitzel, 1976) were used as a starting model for further refinements.

The asymmetric unit contains two cation sites, Sc and Ta, and two O sites, O1 and O2. The Sc site is shared by Sc (dominant) and the impurity elements Sn, Mn, Fe and Ti. The Ta site is occupied by Ta (dominant) and Nb. Although detailed, unrestrained occupancy refinements of the Sc site were tried (with starting values identical to those indicated by the EMPA data), the results were – as expected – inconclusive as to the "true" distribution of the minor impurity elements present. Nonetheless, the Sc site was found to contain somewhat less Sc and more (Sn + Ti + Mn + Fe) than the fragment analysed chemically. The Ta:Nb ratio in the Ta site was also a bit lower by comparison to the EMPA data. However, the structural data clearly confirmed the dominance of Sc and Ta in their respective sites. If all occupancies were fixed according to the EMPA-derived chemical formula [$\sim(Sc_{0.64}Sn_{0.13}Mn_{0.12}Fe_{0.08}Ti_{0.06})_{\Sigma 1.03}(Ta_{0.69}Nb_{0.30})_{\Sigma 0.99}O_4$, with ~25.6 e^- in the Sc site], $R(F)$ was 1.75 %, while unrestrained refinements always led to a lower $R(F)$ of ~ 1.4 % and indicated a formula richer in (Sn + Fe + Mn + Ti), with ~32.3 e^- in the Sc site. For the final model, the occupancy of the Sc site was fixed to the "most probable" values, with the additional constraint of a completely charge-balanced formula (valencies assumed to be Fe^{2+}, Mn^{2+}, Sn^{4+} and Ti^{4+}) and the ratio Ta:Nb was refined freely. This resulted in the formula $(Sc_{0.50}Sn_{0.20}Mn_{0.18}Fe_{0.07}Ti_{0.05})(Ta_{0.58}Nb_{0.42})O_4$. An anisotropic refinement of all atoms led to the final residual $R(F)$ = 1.39 % (further details are provided in Table 2). The final positional and displacement parameters are given in Table 3, and selected bond lengths in Table 4.

Table 2. Crystal data, data-collection information and refinement details for heftetjernite.

Crystal data	
Formula	$(Sc_{0.50}Sn_{0.20}Mn_{0.18}Fe_{0.07}Ti_{0.05})$ $(Ta_{0.58}Nb_{0.42})O_4$
Space group, Z	$P2/c$, 2
a, b, c (Å)	4.784(1), 5.693(1), 5.120(1)
β (°)	91.15(3)
V (Å^3)	139.42(5)
μ (mm^{-1})	28.598
Absorption correction	multi-scan (Otwinowski *et al.*, 2003)
Crystal dimensions (mm)	0.03 × 0.05 × 0.06
Data collection and refinement	
Diffractometer	Nonius KappaCCD system
λ (Mo-$K\alpha$) (Å), T (K)	0.71073, 293
Crystal-detector dist. (mm)	27
Rotation axis, width (°)	ω, 2.0
Total no. of frames	472
Collect. time per degree (s)	77
Collection mode, $2\theta_{max}$ (°)	Full sphere, 70
h, k, l ranges	$-7 \rightarrow 7$, $-9 \rightarrow 9$, $-8 \rightarrow 8$
Total reflections measured	1182
Unique reflections	617 (R_{int} 1.34 %)
Refinement on	F^2
$R1(F)$, $wR2_{all}(F^2)^a$	1.39 %, 3.70 %
"Observed" refls.	607 [$F_o > 4\sigma(F_o)$]
Extinct. coefficient	0.0279(18)
No. of refined parameters	31
GooF	1.188
$(\Delta/\sigma)_{max}$	0.0001
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (e/Å^3)	−1.18, 1.48

Note: Unit-cell parameters were refined from 666 recorded reflections.
Scattering factors for neutral atoms were employed in the refinement.
$^a w = 1/[\sigma^2(F_o^2) + (0.018P)^2 + 0.2P]$; $P = ([\max \text{ of } (0 \text{ or } F_o^2)] + 2F_c^2)/3$.

The atomic arrangement (Fig. 2) is based on two types of edge-sharing, distorted octahedra occupied predominantly by Sc and Ta, respectively. The latter is characterised by a much larger bond-length distortion [range: 1.9024 (18)–2.1293(18) Å] than the former [2.0662 (18)–2.1598 (18) Å]. The bond-angle distortions are similarly strong: the angle values showing the maximum deviation from ideal 90 and 180° angles are 105.95(10) and 161.74(10)° (Sc site) and 76.06(8) and 157.63(11)° (Ta site), respectively.

Table 3. Fractional atomic coordinates and displacement parameters (Å^2) for heftetjernite.

Atom	x	y	z	$U_{\mathrm{eq}}/U_{\mathrm{iso}}$
Sc[a]	0.5	0.67390(6)	0.25	0.00540(15)
Ta[b]	0.0	0.17541(2)	0.25	0.00513(7)
O1	0.2197(4)	0.1076(3)	0.9325(3)	0.0101(3)
O2	0.2644(4)	0.3845(3)	0.4067(3)	0.0097(3)

Note: $U_{\mathrm{eq}} = (1/3) \sum_{\mathrm{i}}\sum_{\mathrm{j}} U_{\mathrm{ij}} a_i * a_j * \mathbf{a_i a_j}$ (Fischer & Tillmanns, 1988).

[a] Occupancy fixed to $\mathrm{Sc_{0.50}Sn_{0.20}Mn_{0.18}Fe_{0.07}Ti_{0.05}}$ (see text).

[b] Refined occupancy: $\mathrm{Ta_{0.580(4)}Nb_{0.420(4)}}$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sc	0.0046(2)	0.0065(2)	0.0051(2)	0.0	0.00044(13)	0.0
Ta	0.00486(9)	0.00506(10)	0.00546(9)	0.0	−0.00057(5)	0.0
O1	0.0101(7)	0.0101(8)	0.0103(7)	−0.0012(6)	0.0001(5)	−0.0010(6)
O2	0.0092(7)	0.0099(7)	0.0098(6)	0.0000(6)	−0.0005(5)	0.0017(6)

Table 4. Selected bond lengths (Å) for the coordination polyhedra in heftetjernite.

Sc–O1 (2x)	2.0662(18)	Ta–O2 (2x)	1.9024(18)
–O2 (2x)	2.0957(18)	–O1 (2x)	1.9913(17)
–O2 (2x)	2.1598(18)	–O1 (2x)	2.1293(18)
<Sc–O>	2.107	<Ta–O>	2.008

Although both synthetic $\mathrm{ScTaO_4}$ and $\mathrm{ScNbO_4}$ are known (see below), their atomic coordinates have been reported only with low precision (Keller, 1962; no *R* values given).

X-ray powder diffraction data were not determined experimentally due to the very small amount of material available; a calculated powder diffraction pattern is given in Table 5, where it is compared with literature data for synthetic $\mathrm{ScTaO_4}$.

6. Discussion

6.1. Isotypic analogues and related minerals

Heftetjernite is isotypic with the tungstates ferberite ($\mathrm{FeWO_4}$), hübnerite ($\mathrm{MnWO_4}$), sanmartinite ($\mathrm{ZnWO_4}$) and synthetic $M^{2+}\mathrm{WO_4}$ (M = Mg, Co, Ni, Zn, Cd). Also isotypic are synthetic $M^{2+}\mathrm{MoO_4}$ (M = Mn, Co, Ni), $\mathrm{MnReO_4}$, $M^{3+}\mathrm{NbO_4}$ (M^{3+} = Fe, In) and $\mathrm{InTaO_4}$. Synthetic wolframite-type $\mathrm{ScTaO_4}$ is well-known (Keller, 1962; Rooksby & White, 1963; Vladimirova *et al.*, 1970; Yokogawa & Yoshimura, 1999). Unit-cell parameters given in the literature ($a = 4.809$, $b = 5.670$, $c = 5.118$ Å, $\beta = 91.67°$, $V = 139.49$ Å^3, Keller, 1962; $a = 4.80$, $b = 5.65$, $c = 5.10$ Å, $\beta = 91.5°$, $V = 138.3$ Å^3, Rooksby & White, 1963; $a = 4.807$, $b = 5.662$, $c = 5.112$ Å, $\beta = 91.62°$, $V = 139.08$ Å^3, ICDD-PDF 24–1017) are similar to those of heftetjernite. A paraelectric-ferroelectric phase transition at 280 ± 1 K of synthetic (flux-grown), light brown, tabular $\mathrm{ScTaO_4}$ crystals was reported by Zhong

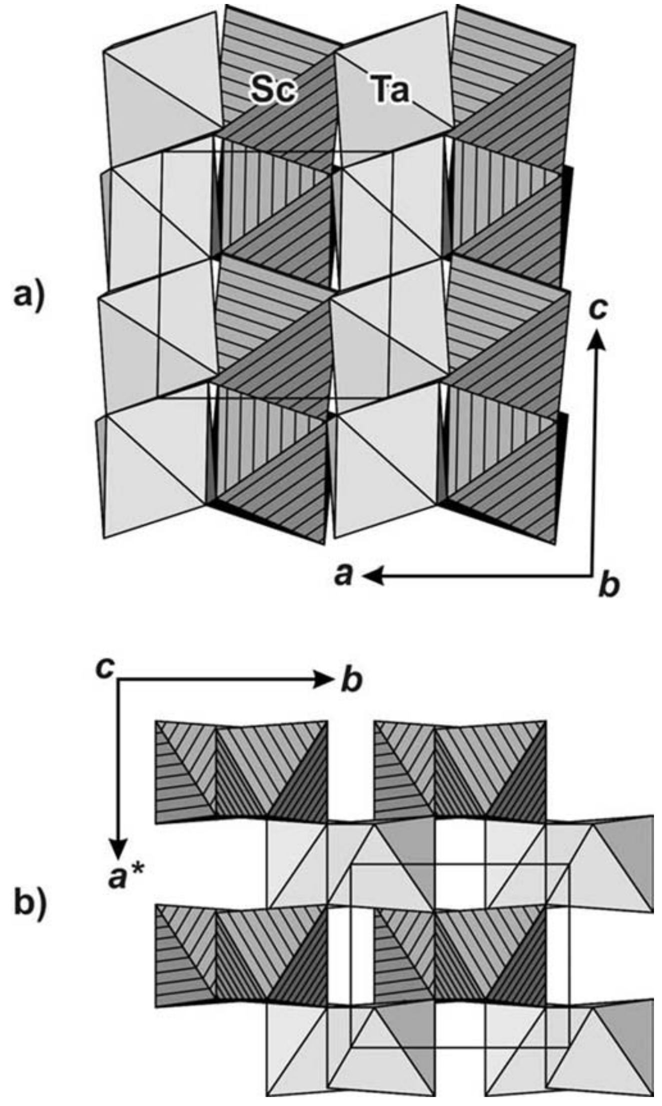

Fig. 2. The crystal structure of heftetjernite in views along (a) the *b*-axis and (b) the *c*-axis. Distorted $\mathrm{ScO_6}$ (striped) and $\mathrm{TaO_6}$ octahedra share common edges. Drawings were done with ATOMS (Shape Software, 1999).

Table 5. Calculated X-ray powder diffraction data for heftetjernite[a], compared with literature data for synthetic $ScTaO_4$.

Heftetjernite (this work)			synthetic $ScTaO_4$ (ICDD-PDF 24–1017)	
I/I_{calc}	d_{calc}	*hkl*	I/I_{meas}	d_{meas}
9	5.693	010	10	5.65
33	4.783	100	45	4.80
32	3.807	01–1	60	3.79
53	3.662	110	50	3.66
100	3.000	11–1	100	3.008
97	2.9570	111	95	2.948
16	2.8465	020	25	2.833
29	2.5595	00–2	35	2.556
34	2.4877	02–1	40	2.477
4	2.4461	120	10	2.439
17	2.3915	200	20	2.402
1	2.3344	01–2	4	2.329
12	2.2758	10–2	25	2.283
1	2.2381	102	6	2.230
2	2.2049	210	8	2.212
18	2.1983	121	35	2.190
8	2.1132	11–2	12	2.117
9	2.0829	112	12	2.075
4	2.0388	21–1	12	2.049
6	2.0115	211	16	2.011
13	1.9032	02–2	20	1.896
3	1.8977	030	–	–
12	1.8311	220	18	1.833
1	1.7755	12–2	–	–
17	1.7652	20–2	25	1.776
27	1.7639	130	35	1.757
2	1.7594	122	–	–
20	1.7325	22–1	25	1.736
15	1.7302	202	20	1.726
22	1.7157	221	25	1.713
1	1.6860	21–2	4	1.694
1	1.6715	13–1	–	–
1	1.6639	131	–	–
1	1.6554	212	–	–
3	1.6345	01–3	8	1.631
1	1.5943	300	6	1.601
15	1.5559	11–3	20	1.558

[a] I/I_{calc} and *hkl* indexing based on a theoretical powder pattern calculated from the refined single-crystal structure.

et al. (1984). Metastable zircon-type $ScTaO_4$ has been grown by the laser-heated pedestal method (Elwell *et al.*, 1985); however, the reported X-ray powder diffraction data (ICDD-PDF 39–29) can not be indexed with the unit cell given by Elwell *et al.* (1985). Synthetic $ScNbO_4$ also has a wolframite-type structure (Schröcke, 1960; Keller, 1962; Rooksby & White, 1963) and may occur in nature (*cf.* Černý *et al.*, 2000; Černý & Chapman, 2001).

The recently described, monoclinic iwashiroite-(Y), $YTaO_4$ (Hori *et al.*, 2006) is not isostructural with heftetjernite, but identical to synthetic M'-type $YTaO_4$ structurally characterised by Wolten (1967) (*cf.* also Wolten & Chase, 1967). Yttrotantalite-(Y) is a metamict (or orthorhombic?) $YTaO_4$ polymorph (Palache *et al.*, 1944; Lima-de-Faria, 1958; Kresten, 1993; *cf.* also Hori *et al.*, 2006), while it is unclear if formanite-(Y), with a composition close to $YTaO_4$, but metamict type material, was tetragonal or monoclinic in its pre-metamict state (Voloshin *et al.*, 2003). The relationships between these yttrium tantalate phases clearly deserve more study.

A Sc-rich variety of ixiolite [ixiolite is orthorhombic (*Pbcn*), cation-disordered $(Ta,Nb,Sn,Fe,Mn)_4O_8$ with a single non-equivalent cation site and a unit cell ($a \sim 4.8$, $b \sim 5.8$, $c \sim 5.2$ Å) being a subcell of the columbite/tantalite and wodginite cells], which was reported by Bergstøl & Juve (1988) from the Heftetjern pegmatite, is a phase chemically similar to heftetjernite. The blackish and shiny mineral sometimes occurs as well-developed rectangular or even square orthorhombic crystals. One of the analyses of Bergstøl & Juve (1988) in fact conforms to a Sc-dominant ''ixiolite'' with $(Sc_{1.46}Ta_{1.16}Nb_{0.76}Sn_{0.26}Fe_{0.24}Mn_{0.18}Ti_{0.03})_{4.09}O_8$ (Raade *et al.*, 2002). Bergstøl & Juve (1988) emphasised that the scandian ixiolite samples are altered (they do not use the term ''metamict'', however), and that some grains are completely altered to metamict members of the pyrochlore group; the degree of alteration ''varies from microscopic areas to a volumetrically complete transformation''. By heating partly altered ixiolite, Bergstøl & Juve (1988) obtained an X-ray powder diffraction pattern of a mixture of pyrochlore (cubic) and wodginite (monoclinic).

We have also identified the rare calcium tantalate rynersonite as an alteration product of ixiolite from Heftetjern; it occurs as golden brown or pale yellow, transparent, rectangular plates in fans up to 1 mm in length, on the surface of strongly altered ixiolite (Kristiansen, 2008).

Wise *et al.* (1998) have discussed the chemical composition and structural behaviour of scandian ixiolite from several localities (including Heftetjern, Mozambique and Madagascar). Scandian ixiolite contains between 4 and 19 wt% Sc_2O_3, and its formula approaches ideal $Sc(Nb,Ta)O_4$. Wise *et al.* (1998) mention an unpublished refinement of the structure of scandian ixiolite [with Ta > Nb according to Table 3 in the paper of Wise *et al.*] from the Heftetjern locality, which indicates that the structure is highly disordered and pseudo-orthorhombic, with a slight departure toward monoclinic symmetry. The monoclinic symmetry of the structure, ''which is apparently related to that of wolframite'', was found to become more obvious after heating. To our knowledge, no structural details (unit cell, space group, etc.) on this anomalously monoclinic scandian ixiolite were subsequently published by Wise and coworkers. Nonetheless, the results of Wise *et al.* (1998) indicate that the very Sc-rich parts of the reported scandian ixiolites from Mozambique and Madagascar (von Knorring *et al.*, 1969) represent a disordered Nb-analogue of the Ta-dominant scandian ixiolite from Heftetjern by Bergstøl & Juve (1988) and Wise *et al.* (1998). Further experimental work on these phases is certainly needed.

The crystal-chemical affinity of Sc for Nb and Ta was already indicated by Goldschmidt & Peters (1931), who explained the presence of scandium in wolframite on the basis of isomorphous replacement of iron and manganese tungstates by scandium niobate or tantalate.

Exsolved scandium-bearing phases in niobian rutile (''ilmenorutile'') from Iveland in southern Norway are potentially new, but so far insufficiently characterised (Černý *et al.*, 2000; Černý & Chapman, 2001). One of them may be identical with a Nb analogue of heftetjernite or closely related to it, since the mineral has the monoclinic $Fe^{3+}NbO_4$ structure type (Černý *et al.*, 2000).

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