Kristiansenite, a new calcium–scandium–tin sorosilicate from granite pegmatite in Tørdal, Telemark, Norway

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With 3 Figures

Summary

Kristiansenite occurs as a late hydrothermal mineral in vugs in an amazonite pegmatite at Heftetjern, Tørdal, Telemark, Norway. Tapering crystals, rarely up to 2 mm long, are colourless, white, or slightly yellowish. The mineral has the ideal composition $Ca_2ScSn(Si_2O_7)(Si_2O_6OH)$ and is triclinic $C\bar{1}$ with cell parameters $a = 10.028(1)$, $b = 8.408(1)$, $c = 13.339(2)$ Å, $\alpha = 90.01(1)$, $\beta = 109.10(1)$, $\gamma = 90.00(1)°$, $V = 1062.7(3)$ Å^3 $(Z = 4)$. It has a monoclinic cell within ~ 0.1 Å and is polysynthetically twinned on {010} by metric merohedry. The strongest reflections in the X-ray powder pattern are [d in Å, (I_{obs}), (hkl)]: 5.18 (53) (1–11), 3.146 (100) (004), 3.089 (63) (−222), 2.901 (19) (221), 2.595 (34) (222), 2.142 (17) (−3−31). The Mohs' hardness is 5½–6; $D_{calc.} = 3.64$ g/cm^3; only a mean refractive index of 1.74 could be measured. Scandium enrichment in the Heftetjern pegmatite and the crystal chemistry of scandium are briefly discussed.

Introduction

Scandium is not one of the rarest elements in the Earth's crust, e.g. it is about ten times more abundant than tin. However, it is a dispersed element in the lithosphere and the great bulk of it is contained in ferromagnesian minerals. This explains the scarcity of minerals in which scandium occurs as an essential constituent. Prior to

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the present description only eight scandium minerals were known (with year of first description): thortveitite [$(Sc,Y)_2Si_2O_7$] (1911), bazzite [$Be_3(Sc, Al)_2Si_6O_{18}$] (1915), kolbeckite [$ScPO_4 \cdot 2H_2O$] (1926; not originally recognised as a scandium mineral), jervisite [$(Na, Ca, Fe^{2+})(Sc, Mg, Fe^{2+})Si_2O_6$] and cascandite [$Ca(Sc, Fe^{2+})Si_3O_8(OH)$] (described in the same paper, 1982), juonniite [$CaMgSc(PO_4)_2(OH) \cdot 4H_2O$] (1997), pretulite [$ScPO_4$] (1998), and scandiobabingtonite [$CaFe^{2+}ScSi_5O_{14}(OH)$] (1998). As can be seen, five of these minerals were described within the last two decades.

The description of kristiansenite [$Ca_2ScSn(Si_2O_7)(Si_2O_6OH)$] from the Heftetjern granite pegmatite in the Tørdal area (Telemark, Norway) brings the total number of scandium minerals to nine. The extreme enrichment of scandium in this pegmatite is discussed below. The prospects of finding other new minerals with scandium as a major element in the Heftetjern pegmatite seem to be good.

Kristiansenite is named for Mr. *Roy Kristiansen* (1943-), a well-known amateur mineralogist from Norway who first noticed the new mineral. The Commission on New Minerals and Mineral Names (IMA) has approved the mineral and its name (2000-051). Type material is lodged at the Geological Museum, University of Oslo.

The Tørdal area and the Heftetjern pegmatite

The Tørdal area in Telemark is geochemically different from the other granite pegmatite areas in south Norway, being characterized by tin, scandium, and lithium. Amazonite-cleavelandite pegmatites in Høydalen and at Skarsfjell were described by *Oftedal* (1942), cf. *Raade* et al. (1993). Here lithium occurs in lepidolite and zinnwaldite, and tin in cassiterite. Other characteristic elements are beryllium [beryl, gadolinite-(Y)], niobium/tantalum and rare earth elements [e.g. fergusonite-(Y), yttrotantalite-(Y), microlite, monazite-(Ce), allanite-(Ce), kuliokite-(Y)]. Also a high fluorine level is conspicuous [yttrian fluorite, tveitite-(Y), kuliokite-(Y), topaz].

The Heftetjern amazonite pegmatite is situated between Skarsfjell and Høydalen. The mineralogy of this pegmatite and the general geology of the area were described by *Bergstøl* and *Juve* (1988) and *Juve* and *Bergstøl* (1990). A striking geochemical feature of the Heftetjern pegmatite, already noted in these two papers, is the high level of scandium. Also beryllium and tin are characteristic elements, but lithium and fluorine to a much lesser degree.

The numerous granite pegmatites of the Tørdal area 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* and *Juve*, 1988). Rb–Sr dating of lepidolite and microcline from the Skarsfjell pegmatite gave ages between 950 and 880 Ma (*Neumann*, 1960; *Mitchell*, 1967). From trace-element analyses of different rock types it has been suggested that some of the tin and a major part of scandium 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* and *Juve*, 1988).

Bazzite, scandian ixiolite, and scandian members of the pyrochlore group – formed by late hydrothermal alteration of scandian ixiolite – were described by

Bergstøl and *Juve* (1988) and a cesian bazzite with 3 wt.% Cs_2O by *Juve* and *Bergstøl* (1990). The empirical formula of the ixiolite with highest scandium content (18.80 wt.% Sc_2O_3) is $(Sc_{1.46}Ta_{1.16}Nb_{0.76}Sn_{0.26}Fe_{0.24}Mn_{0.18}Ti_{0.03})_{\Sigma4.09}O_8$. Ixiolite ideally has a structure with disordered cations and this could in fact be a new species. Whether scandium in ixiolite is disordered over all three cation sites or not needs further study (cf. *Wise* et al., 1998). Ixiolite from Mosambique with only 6.00 wt.% Sc_2O_3 was proclaimed as the new species ''scandium ixiolite'' by *Borisenko* et al. (1969); however, this name has no standing.

The scandium minerals cascandite (*Mellini* et al., 1982) and scandiobabingto-nite (*Orlandi* et al., 1998) were recently identified from the Heftetjern pegmatite. In one case the two minerals occurred in a fibrous state and were found to be intimately intergrown (*Raade* and *Erambert*, 1999). This is not surprising since both are pyroxenoids, cascandite with a *dreier* chain and scandiobabingtonite with a *fünfer* chain of SiO_4 tetrahedra.

The unusual enrichment of scandium in the Heftetjern pegmatite is not only manifested in the occurrence of several minerals with scandium as a main constituent but also in high levels of the element in other minerals. By EDX analyses we have measured approximate scandium contents (as wt.% Sc_2O_3) in the following minerals: ferrotantalite (~ 7), ilmenorutile (~ 1.6), spessartine (~ 0.3), epidote (~ 2.0), helvite (~ 1.3), and milarite (5–7). Detailed paragenetic studies and determination of the scandium content of other minerals are planned for the future. So far, the scandium-bearing minerals in the Heftetjern pegmatite seem to be confined to a late hydrothermal phase of pegmatite formation.

Appearance and physical properties

Kristiansenite occurs as tapering crystals rarely up to 2 mm long (Fig. 1) and was also observed as a massive aggregate nearly 2 mm across. It shows twin striations from polysynthetic twinning on {010}. The complex crystals were not suited for goniometric measurements due to twinning, small size, and mostly dull faces. The mineral is colourless, white or slightly yellowish with a white streak. It is
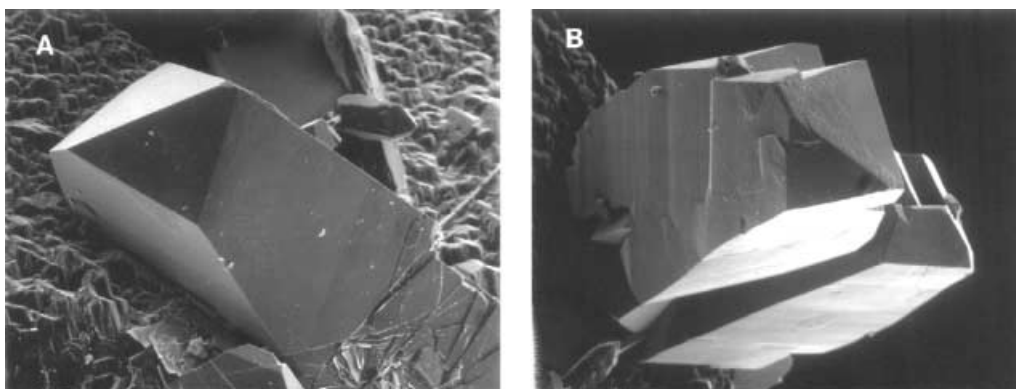

Fig. 1. SEM images of kristiansenite. The single crystal (**A**) is ~ 0.2 mm long; the crystal group (**B**) is ~ 0.3 mm long

translucent to transparent and has a vitreous lustre. Fluoresence was not observed, nor any cleavage or parting. However, the enhancement of the (004) reflection in the X-ray powder patterns could indicate a certain degree of preferred orientation from a {001} cleavage (see below). The density is above $3.3\,g/cm^3$ (the mineral sinks in di-iodomethane). The calculated density is $3.64\,g/cm^3$. The Mohs' hardness is $5\frac{1}{2}$ to 6. The mineral is brittle and has an uneven fracture.

Precise indices of refraction were impossible to determine. Even in very small grains, the fragments are intensively twinned and show extreme undulatory extinction. The only optical property that could be measured was a mean refractive index $n = 1.74$.

Occurrence

Kristiansenite is most closely associated with quartz, albite, apatite, biotite, and stilpnomelane. Other minerals on the kristiansenite samples are scandiobabingtonite, scandian ixiolite, hingganite-(Y), cerian epidote, titanite, plumbomicrolite and other microlite minerals, bazzite, and milarite. In one case kristiansenite was found along a crack in cassiterite with two unidentified tantalum minerals (rynersonite?, tantite?). It is a late-stage hydrothermal mineral in pegmatite vugs, formed later than albite and earlier than a latest generation of tiny quartz crystals.

Chemical data

Electron microprobe analyses were made on several grains and in three different laboratories (Table 1). Wavelength-dispersive analyses on grains SN1, SN2, and SN3 (the latter is the one used for crystal structure work) were performed at Modena University on an ARL-SEMQ electron probe at 15 kV and 20 nA with 10 s counting time. The probe standards were albite (Na), microcline (K), clinopyroxene (Ca, Si), spessartine (Al), ilmenite (Fe, Ti), SnO_2 (Sn), metallic Sc and Zr. Samples A and B, analysed in wavelength-dispersive mode on a Cameca Camebax electron probe in Oslo, gave very similar results and the values have been averaged in Table 1. The measurements were made at 15 kV and 17 nA with 10 s counting time (20 s for Al) using the following standards: wollastonite (Ca, Si), Fe_2O_3 (Fe), $MnTiO_3$ (Ti), Al_2O_3 (Al), SnO_2 (Sn), and Sc_2O_3 (Sc). Nb was measured separately as a trace element with Nb metal as standard, using 60 s counting time. An SEM JEOL JSM-6310 instrument with attached EDX Oxford Link Isis was used in Graz on sample 65b, being operated at 15 kV and 5 nA with 100 s counting time. The standards were: garnet (Si, Al, Fe), titanite (Ca, Ti), $ScPO_4$ (Sc), and SnO_2 (Sn).

All the analyses close at a sum that is slightly below 100 wt.%. According to the crystal structure data (*Ferraris* et al., 2001) the mineral contains hydroxyl groups. H_2O was not determined directly due to a combination of low content and dearth of material. Adding 2.04 wt.% H_2O to the analysis of sample SN3 (used for structure work) to bring the sum to 100%, the following empirical formula is obtained for that sample, based on $7(O + OH)$: $(Ca_{0.96}Na_{0.04})_{\Sigma1.00}(Sn_{0.53}Sc_{0.34}Fe_{0.07}Al_{0.02}Zr_{0.01})_{\Sigma0.97}Si_{1.98}(O_{6.34}OH_{0.66})_{\Sigma7.00}$. Alternatively, normalizing the empirical formula on the basis of 2Si gives $(Ca_{0.97}Na_{0.04})_{\Sigma1.01}(Sn_{0.53}Sc_{0.35}Fe_{0.07}Al_{0.02}Zr_{0.01})_{\Sigma0.98}Si_{2.00}(O_{6.41}OH_{0.67})_{\Sigma7.08}$. The simplified formula, taking into

Table 1. *Electron-microprobe analyses of kristiansenite*

	SN1		SN2		SN3		A/B dark area		A/B light area		65b	
	M(9)	Range	M(7)	Range	M(11)	Range	M(6)	Range	M(6)	Range	M(10)	Range
Na_2O	0.00	–	0.04	0.00–0.08	0.41	0.14–0.82		n.a.		n.a.		n.a.
K_2O	0.00	–	0.00	–	0.06	0.00–0.18		n.a.		n.a.		<0.10
CaO	19.27	18.97–19.51	19.35	18.84–19.74	18.45	17.88–19.06	19.43	19.23–19.67	19.22	18.97–19.45	18.80	18.38–19.28
Al_2O_3	0.40	0.29–0.54	0.44	0.30–0.65	0.35	0.23–0.61	0.49	0.40–0.57	0.51	0.31–0.62	0.27	<0.22–0.54
Sc_2O_3	8.47	7.47–9.70	7.79	6.87–9.32	8.11	7.38–8.91	9.74	9.31–10.13	8.34	8.06–8.73	9.55	9.23–10.21
Fe_2O_3	3.04	2.24–4.33	2.68	2.14–3.57	1.98	1.62–3.11	2.26	1.96–2.59	2.61	2.06–3.01	1.53	0.90–2.20
SiO_2	41.08	40.17–41.64	40.84	39.90–41.66	40.76	40.14–41.97	40.90	40.60–41.26	40.23	39.96–40.63	40.16	39.19–41.19
TiO_2	0.15	0.00–0.44	0.09	0.06–0.21	0.08	0.03–0.11	0.42	0.40–0.46	0.15	0.12–0.20		<0.16
ZrO_2	0.28	0.03–0.49	0.34	0.19–0.56	0.43	0.20–0.69		n.a.		n.a.		n.a.
SnO_2	25.67	24.15–26.85	27.33	25.97–28.29	27.33	25.30–28.85	24.37	23.95–24.75	25.69	25.21–26.39	26.52	25.55–27.25
Nb_2O_5	0.11	0.00–0.53	0.00	–	0.00	–	0.16*	0.11–0.19	0.84**	0.50–1.03		n.a.
H_2O					2.04***							
Sum	98.47		98.90		100.00		97.77		97.59		96.83	

M mean (number of analyses in parenthesis), *n.a.* not analysed, * mean of 3 analyses, ** mean of 4 analyses, *** by difference, SN3 is the crystal that was used for structure determination
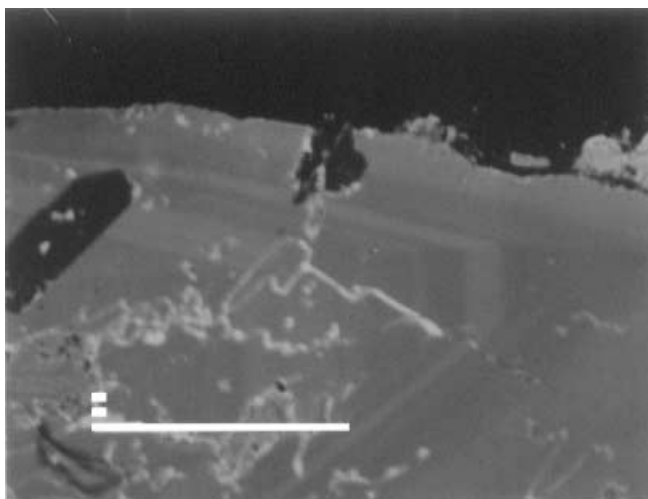
Fig. 2. Oscillatory zonation in a kristiansenite crystal (sample AH4). Backscatter image; scale bar is 100 μm. The black prism to the left is an apatite crystal

consideration the crystal structure data, is $Ca_2ScSn(Si_2O_7)(Si_2O_6OH)$, which requires CaO 19.30, Sc_2O_3 11.86, SiO_2 41.36, SnO_2 25.93, H_2O 1.55, total 100.00 wt.%. In all the analyses the percentages required to bring the totals to 100% are close to the expected wt.% value of H_2O.

The Gladstone-Dale relationship, based on the above empirical composition and using the calculated density, gives a compatibility index of -0.024, which is excellent (*Mandarino*, 1981).

Backscatter images often show irregular or oscillatory zoning in kristiansenite crystals (Fig. 2). For the samples A and B, analyses of darker and lighter areas on the backscatter images were treated separately (Table 1). The main feature is: higher contents of Sc and Ti and lower contents of Sn and Nb in the darker areas. The analyses of A/B samples when separated into dark and light areas have narrower ranges for most elements as compared to the other mean analyses in Table 1. This would indicate zonation in the other analysed samples as well.

X-ray powder diffraction data

The X-ray powder diagram (Table 2) was recorded with a Siemens D5005 diffactometer, using a curved graphite secondary monochromator and $CuK\alpha_1$ radiation. The calibration standard was quartz. Indexing was done by taking into account the diffraction intensities calculated from the crystal structure. The indices which are equivalent according to the pseudo-monoclinic symmetry are not reported. The overall agreement between observed and calculated intensities is good, except for an enhancement of the (004) reflection in the observed patterns. This could perhaps be due to some degree of preferred orientation resulting from a {001} cleavage, which is otherwise unnoticed. It turns out that a {001} cleavage is reasonable because that plane exactly intersects the hydrogen bonds and cuts only a small number of the cation-oxygen coordination bonds (cf. Fig. 1 in *Ferraris* et al., 2001). Cell parameters refined from powder data are: $a = 10.007(5)$, $b = 8.401(5)$, $c = 13.327(5)$ Å, $\alpha = 90.08(4)$, $\beta = 109.06(3)$, $\gamma = 90.01(4)°$, $V = 1058.9(6)$ Å^3.

Table 2. *X-ray powder diffraction data for kristiansenite*

I_{obs}	I_{calc}	d_{obs} (Å)	d_{calc} (Å)	h	k	l
11	8	6.27	6.28	−1	1	0
4	11	6.17	6.18	−1	1	1
53	49	5.18	5.19	1	−1	1
6	9	4.71	4.73	2	0	0
10	23	4.55	4.56	−2	0	2
12	13	3.898	3.906	−1	−1	3
8	14	3.209	3.215	−2	−2	1
100	57	3.146	3.149	0	0	4
63	100	3.089	3.090	−2	2	2
19	26	2.901	2.902	2	2	1
10	12	2.824	2.827	−2	−2	3
34	41	2.595	2.593	2	2	2
6	16	2.365	2.365	4	0	0
8	17	2.207	2.204	−2	0	6
17	30	2.142	2.141	−3	−3	1
9	12	2.060	2.061	−4	2	0
7	13	2.007	2.006	−4	−2	4
8	16	1.951	1.953	−2	−2	6
8	15	1.878	1.877	0	4	3
7	5	1.837	1.838	−1	1	7
7	9	1.813	1.814	−3	3	5
11	12	1.731	1.729	3	3	3
6	12	1.680	1.679	3	1	5
6	16	1.620	1.619	−5	3	3
7	15	1.547	1.546	−6	2	2
12	11	1.433	1.434	1	3	7
7	13	1.382	1.381	−5	3	7
8	10	1.350	1.349	1	−5	5
8	5	1.298	1.298	4	−2	6

Crystal structure

The structure of kristiansenite has been solved and refined anisotropically from a crystal that is polysynthetically twinned on {010} by metric merohedry; it is fully described by *Ferraris* et al. (2001) and here only the main features are reported. The final R1 is 0.0242 for 4862 observed reflections. The space group is $C\bar{1}$ with cell parameters $a = 10.028(1)$, $b = 8.408(1)$, $c = 13.339(2)$ Å, $\alpha = 90.01(1)$, $\beta = 109.10(1)$, $\gamma = 90.00(1)°$, $V = 1062.7(3)$ Å^3 ($Z = 4$). The triclinic structure approximates monoclinic symmetry within ~ 0.1 Å in the atomic positions.

The structure (Fig. 1 in *Ferraris* et al., 2001) contains Si_2O_7 double tetrahedra (sorosilicate or disilicate groups) and isolated polyhedra of 6-coordinated Sn, Sc, Fe and $(7+2)$-coordinated Ca cations. Taking into account the chemical analysis and the refined number of electrons per site, *Ferraris* et al. (2001) proposed the following compositions for the octahedral M sites: $M1 = 0.99Sn + 0.01Fe$; $M2 = 0.61Sn + 0.39Sc$; $M3 = 0.30Sn + 0.50Sc + 0.20Fe$; $M4 = 0.17Sn + 0.63$

Sc + 0.20Fe. Half of the disilicate groups carry a hydrogen atom; thus kristiansenite is the first known case with the presence of both protonated Si_2O_6OH and normal Si_2O_7 disilicate groups and represents a new type of silicate structure. The octahedra M are isolated from each other and alternate with the disilicate groups along $(10\bar{1})$ planes. Two independent and relatively short $O \cdots O$ hydrogen bonds connect [101] rows of sorosilicate groups and are discussed below.

Infra-red spectrum and hydrogen bonding

The IR spectrum was measured with a Perkin-Elmer AutoIMAGE System FT-IR microscope (Fig. 3). The mineral powder dispersed in a KBr disc gave well-resolved absorption bands below $1400\,cm^{-1}$ (at 1218, 986, 938, 846, and $717\,cm^{-1}$). According to the empirical correlation between O–H stretching frequencies and O–H $\cdots$ O hydrogen bond lengths in minerals by *Libowitzky* (1999) the two O $\cdots$ O distances of $2.645(7)\,\text{Å}$ (O11 $\cdots$ O2) and $2.627(9)\,\text{Å}$ (O21 $\cdots$ O28), representing hydrogen bonds in the kristiansenite structure (*Ferraris* et al., 2001), would be expected to give O–H stretching bands at ~ 2980 and $\sim 2890\,cm^{-1}$, respectively. Two small but distinct absorption bands at 2924 and $2854\,cm^{-1}$ in the IR spectrum are remarkably close to these values. However, these two bands are apparently related to C–H stretching modes of organic impurities. Presumably the O–H stretching bands are buried in the broad bump appearing in the range ~ 3000–$2700\,cm^{-1}$.

From the structural results published by *Ferraris* et al. (2001) it turns out:

1. the difference in the bond valences, calculated without the hydrogen contribution, between (supposed) donor (O11: −1.40; O21: −1.42) and (supposed) acceptor (O2: −1.68; O28: −1.52) oxygen atoms is small;
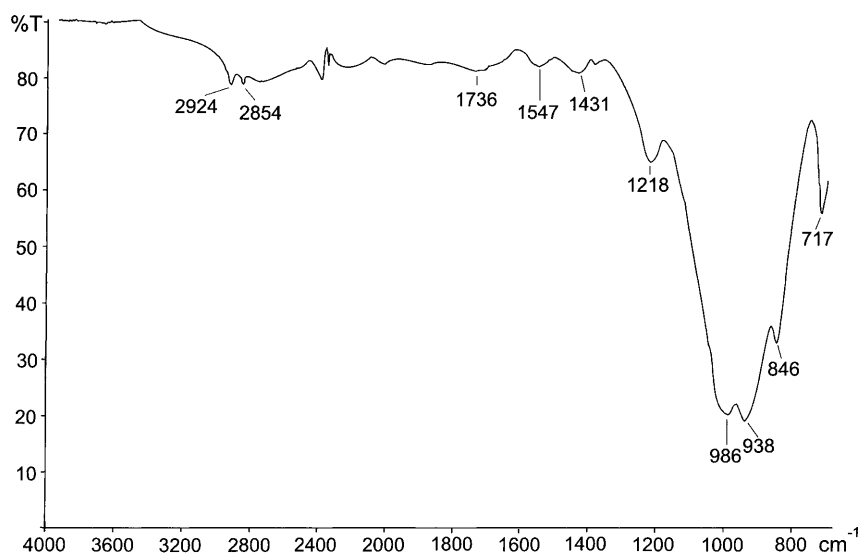

Fig. 3. Infra-red spectrum of kristiansenite (in KBr disc). The abscissa shows the wavenumber in cm^{-1} and the ordinate is the transmittance in %

2. there is a small difference in length between the Si–O bonds, while Si–OH bonds are expected to be clearly longer than Si–O bonds (*Ferraris* and *Ivaldi*, 1984);
3. the hydrogen atoms were not detected in the difference electron density map.

From these features it could be concluded that some degree of disorder affects the two protons involved in hydrogen bonding. That would mean a mixed donor/acceptor role of the involved oxygen atoms and a range of O–H bond lengths, thus explaining the mentioned broad IR stretching band.

Crystal chemistry of scandium

Incorporation of scandium in minerals is a complex matter. Scandium and yttrium have fundamental similarities in the outer electron structure to each other and to the rare earth elements and both have been classed with the latter elements. However, the relatively small size of the Sc^{3+} ion (in 6-coordination $0.745\,\text{Å}$ as compared to $0.900\,\text{Å}$ for Y^{3+} and $0.868\,\text{Å}$ for Yb^{3+}; *Shannon*, 1976) is responsible for a number of other homo- and heterovalent substitutions.

The most common substitution involving scandium is the replacement of aluminium and trivalent iron:

$$Sc^{3+} = (Al, Fe^{3+}).$$
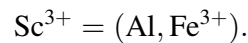
This is the main reason for the dispersal of scandium in the lithosphere and it explains the high scandium contents of minerals like spessartine, epidote, and milarite mentioned above. It also indicates that there may be scandium analogues of many Al, Fe^{3+} minerals.

Thortveitite $[(Sc, Y)_2Si_2O_7]$, keiviite-(Y) $[(Y, Yb)_2Si_2O_7]$, and keiviite-(Yb) $[(Yb, Y)_2Si_2O_7]$ are isotypic, which involves another simple scandium substitution, in spite of a rather large difference in ionic radii:

$$Sc^{3+} = (Y, Yb)^{3+}.$$
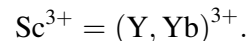
Incorporation of scandium in Nb, Ta minerals is best explained by the coupled substitution (*Novák* and *Černý*, 1998; *Wise* et al., 1998):

$$Sc^{3+} + (Ti, Sn)^{4+} = (Fe, Mn)^{2+} + (Nb, Ta)^{5+}.$$
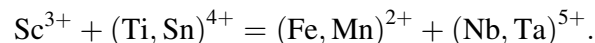
Pretulite $[ScPO_4]$ with a zircon-type structure was described as a new mineral by *Bernhard* et al. (1998). A scandium phosphate with $13–24\,\text{mol\%}$ $ZrSiO_4$ was analysed by *Novák* and *Šrein* (1989). This shows that there is a series between pretulite and zircon, involving a coupled substitution of the type:

$$Sc^{3+} + P^{5+} = Zr^{4+} + Si^{4+}.$$
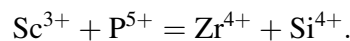
Jervisite $[(Na, Ca, Fe^{2+})(Sc, Mg, Fe^{2+})Si_2O_6]$ (*Mellini* et al., 1982) is a pyroxene and the following coupled substitution is involved:

$$Sc^{3+} + Na^+ = (Mg, Fe)^{2+} + Ca^{2+}.$$
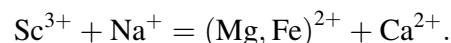
The elevated content of scandium in helvite, mentioned above, could be due to a coupled substitution of the type:

$$Sc^{3+} + Al^{3+} = (Mn, Fe, Zn)^{2+} + Si^{4+}.$$

However, aluminium is below the detection limit (0.18 wt.% Al_2O_3) in this mineral. Another possibility could involve vacancies:

$$2Sc^{3+} + 1\square = 3(Mn, Fe, Zn)^{2+}.$$
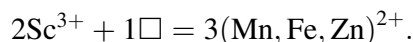
This possiblity is intended to be investigated more closely.

Finally, the $(Sc + Fe + Al):Sn$ ratio of kristiansenite is close to unity. Accordingly, a completely ordered structure with respect to Sc and Sn would be expected. However, as reported above, these elements are only partially ordered: Sn completely fills $M1$, subordinately enters $M2$, and, to a lesser degree, $M3$ and $M4$; conversely, Sc (and the small amount of Fe) preferentially enters $M4$ and $M3$ and to a lesser degree $M2$. A similarity of ionic radii for 6-coordination makes this substitution feasible, Sc^{3+} having a radius of 0.745 Å and Sn^{4+} a radius of 0.690 Å (*Shannon*, 1976). In conclusion, the distribution of Sn^{4+} cations on all four M sites, instead of a concentration on only two of the sites, is allowed in terms of ionic radii and is reasonably a matter of bond valence balance.

The minor surplus of Sn over $(Sc + Fe + Al)$ in the empirical formula of the kristiansenite sample SN3, which is in accordance with the occupancy refinement of that sample (*Ferraris* et al., 2001), is balanced by a replacement of Na for Ca according to the scheme:

$$Sn^{4+} + Na^+ = (Sc, Fe, Al)^{3+} + Ca^{2+}.$$

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