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Crystal chemistry of two tourmalines from Høydalen, Tørdal, Telemark, Norway

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Introduction

Tourmalines or, strictly speaking, the members of the tourmaline supergroup, occur in many rock types and can show an intriguing variability of their crystal chemistry. From a crystal-structural point of view, tourmalines are classified as cyclosilicates. Their atomic arrangement is characterised by one tetrahedrally coordinated *T* site, predominantly occupied by Si with lesser amounts of Al. Six TO_4 tetrahedra form a $[T_6O_{18}]$ ring by corner-sharing. A triangularly coordinated site is occupied by boron, $[BO_3]$. There are two sites in octahedral coordination, *Y* and *Z*, and an *X* site that is nine-coordinated. Thus, the general chemical formula of tourmaline minerals can be written as

$XY_3Z_6[T_6O_{18}][BO_3]_3V_3W$, where the most common constituents are:

$X = Na, Ca, \square$ (vacancy)

$Y = Fe^{2+}, Mg, Mn^{2+}, Al, Fe^{3+}, Li, Ti$

$Z = Al, Fe^{3+}, Mg$

$T = Si, Al$

$V = OH, O$

$W = OH, F, O$

In addition, Cr^{3+} and V^{3+} may occur in species-defining amounts at the *Y* and *Z* sites in some rare cases.

This chemical complexity gives rise to a number of different species in the tourmaline supergroup, for which a new IMA-approved nomenclature was recently published (Henry *et al.* 2011). Subsequent to its publication, a number of new species has been approved and described. The most recent edition of *Fleischer's Glossary of Mineral Species* (Back 2014) lists 24 tourmaline species, whereas mindat.org in January 2016 has 34 species.

There has been a flood of papers in recent years dealing with different aspects of tourmalines. Special sessions on tourmaline have been arranged at international meetings, and the October 2011 issue of the *Elements* magazine was entirely devoted to the subject. This was also the case for the February 2011 issue of *The Canadian Mineralogist*, entitled “Tourmaline: An ideal indicator of its host environment” (405 pages). The main topics included “Crystallography and crystal chemistry of tourmaline”, “Tourmaline stability and element partitioning” and “Tourmaline as a petrogenetic

indicator”. Tourmalines are widespread in a wide variety of rocks, and their composition reflects a large diversity in terms of chemical environment, temperature and pressure.

Tourmaline is relatively rare in the Høydalen granitic pegmatites and has not previously been studied. The two samples reported on here were investigated with the main purpose of establishing their compositions. Since they occur with different mineral associations, a comparison of their crystal chemistry would seem to be of interest.

Occurrence

The internal structure and mineralogy of the granitic pegmatites at Høydalen were described by Oftedal (1942). These complex pegmatites cut through coarse-grained metamorphosed gabbro of Precambrian age. Neumann (1960) has reported Rb-Sr ages averaging 910 Ma for lepidolite and microcline from these pegmatites. Primary amazonite pegmatites are to a large extent replaced by a cleavelandite phase. Quarrying for lepidolite, amazonite and mineral specimens for collectors (like cassiterite, beryl, topaz, gadolinite-(Y), etc.) has taken place in two pegmatites situated a few hundred metres apart, called the upper and lower quarries; both are now abandoned. The two specimens studied here come from the upper quarry. The pegmatite dike is here about 5 m thick with nearly E-W strike and varying dip close to vertical. Some geochemical aspects relating to the process of replacement of amazonite pegmatite by cleavelandite pegmatite in the Høydalen area have been discussed by Oftedal (1956). Kristiansen (1998) has provided a chronological survey of publications and events related to the Høydalen pegmatites, and an updated list of minerals was published by Segalstad & Raade (2003).

The Tørdal pegmatites belong to the mixed LCT (with Li, Cs, Ta) – NYF (with Nb, Y, F) rare-element petrogenetic family of Černý (1991). The Høydalen pegmatites have a distinct Li, F, Y, Ta signature with additional Be and Sn. They classify as lepidolite-subtype pegmatites (Černý 1991). Černý & Ercit (1985) write about the Høydalen pegmatites: “Evidently a strong Y, REE signature of the whole pegmatite district persists through advanced fractionation into the Li, F-enriched, lepidolite-bearing pegmatite type”.

Sample descriptions

Tourmaline in sample RK (collected by Roy Kristiansen on the mine dump) is dark olive brown and is embedded in coarse albite-quartz graphic granite. The two main parts of the mineral occur as columnar, broken aggregates 0.7 and 1.5 cm long; these are remnants of an originally larger mass. The tourmaline has contacts to both smoky quartz and albite. One end of the specimen is quartz-free and consists of platy albite (cleavelandite) with a 1 cm large inclusion of deep-green gadolinite-(Y).

Coarse albite and smoky quartz are the main phases also of the GR specimen (collected by the first author on the mine dump) which is cut by a thin layer carrying pale green muscovite (polytype $2M_1$), white to colourless beryl and tourmaline. The beryl may form patches up to 2 cm across. Tourmaline occurs as scattered green to bluish green prismatic aggregates up to 0.5 cm long, embedded in both muscovite and beryl and occasionally also in contact with albite and quartz. There is no cleavelandite in this sample.

Analytical details

Electron probe microanalyses (EPMA) in wavelength-dispersive mode were performed on standard polished and carbon-coated grain mounts with a Cameca SX100 instrument (measurement conditions: 15 kV acceleration voltage, 15 nA beam current, beam spot size 5 μm). An EDS scan revealed the presence of Si, Al, Fe, Mn, Mg and Na. In addition, minor amounts of K, Ca, Ti and F were detected by WDS scans. Zn, Sc and Cr were sought but not found. The probe standards were: albite (Na), orthoclase (K), MgO (Mg), wollastonite (Ca and Si), pyrophanite (Mn and Ti), Fe metal (Fe), Al_2O_3 (Al) and fluorite (F). All elements were analysed using $K\alpha$ lines. A total of 13 spots were analysed on two grains of sample GR, and 9 spots on three grains of sample RK. The F content initially varied erratically from zero to in excess of 1 wt%, indicating a problem with the spectrometer crystal, and had to be reanalysed separately at a later date, using a LTAP crystal. For matrix correction, element percentages from one selected data set of the previous analyses of each of the GR and RK samples plus 3.05 wt% B for sample RK and 3.10 wt% B for sample GR were applied. These B values are preliminary ICP-MS results (see below) which later, compared to calculated values for B_2O_3 , based on 6 Si a.p.f.u. (atoms per formula unit), turned out to be slightly on the low side. For sample RK, 18 new F analyses were performed and 12 for sample GR. Back-scattered electron (BSE) images revealed weak and irregular zonation in one of the GR grains, dependent on variations in Fe content. No zonation was seen in the RK grains. No inclusions were observed in either sample.

The light elements Li and Be were determined by inductively coupled plasma mass spectrometry (ICP-MS) using a PerkinElmer Elan DRC II instrument (STD Mode). The samples were finely ground in an agate mortar under absolute alcohol. Dry aliquots of each sample (14.3 mg of GR and 13.5 mg of RK) were decomposed in a microwave-assisted closed system with HF and HNO_3 .

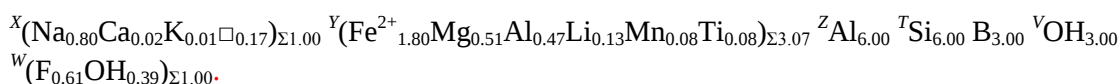
The crystal structures of both RK and GR were determined at ambient temperature with a Nonius KappaCCD single-crystal X-ray diffractometer using graphite-monochromated $\text{MoK}\alpha$ radiation. Highly redundant data were collected for an approximate sphere of reciprocal space and were integrated and corrected for Lorentz and polarization factors and absorption (Otwinowski *et al.* 2003). The structures were refined with *SHELXL-97* (Sheldrick 2008) using scattering factors for neutral atoms and the structure model from Fortier & Donnay (1975) as a starting model. During all initial refinements, the X site was modelled with Na scattering factors and unconstrained occupancy, and the Y site and Z site were similarly modelled using Al and Fe scattering factors. The T site was modelled using Si scattering factors, but with fixed occupancy of $\text{Si}_{1.00}$, because refinement with unconstrained occupancy showed this site to be essentially fully occupied by Si within error limits. The B site was modelled with fixed occupancy of $\text{B}_{1.00}$. The H site was freely refined, as was the F:O ratio on the W site. For the final refinement steps, the model was adjusted to the chemical composition obtained from the EPMA data (for details see below). Selected crystal data, data collection information and refinement details for the two samples are given in Table 1. CIF files with atomic coordinates and displacement parameters are available from the second author and will be submitted to the Inorganic Crystal Structure Database.

Results

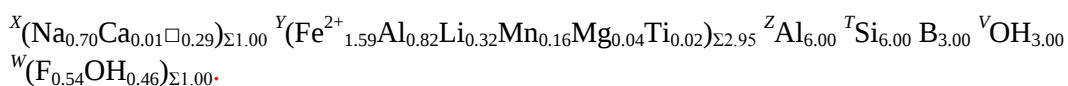
Chemical analytical data are presented in Table 2. Iron is assumed to be divalent. The quantities of B_2O_3 and H_2O were not determined and are calculated on the basis of Si = 6 a.p.f.u. to give 3 B a.p.f.u. and 4 (OH+F) a.p.f.u. This excludes any oxy component on the V and W sites. The resulting

analytical totals are very reasonable (100.82 for RK and 100.32 for GR). Interference of the $FK\alpha$ line with Fe and Mn $L\beta$ lines can be corrected for by using the equation $F = F_{\text{meas}} - (-0.000055\text{FeO}^2 + 0.00889\text{FeO} - 0.0044) + 0.015\text{MnO}$ (Kalt *et al.* 2001; 0.0889FeO in the paper is a misprint). Applying this correction to the F values in Table 2 yields 1.06 and 0.95 wt% for RK and GR, respectively, corresponding to 0.57 and 0.50 F a.p.f.u. These corrected values have not been included in Table 2, since the accuracy of the listed figures is probably relatively poor because the F peak height was measured instead of considering the peak area. The BeO content was determined by ICP-MS and was below the detection limit (< 0.003 wt%) for sample RK and as high as 0.108 wt% for sample GR. The GR tourmaline partly occurs embedded in beryl, and although the utmost care was taken to select pure material, it is likely that the measured BeO in GR, all or for the most part, is caused by contamination. It is therefore not included in Table 2. Novák *et al.* (2011) have reported Be contents up to 31.5 ppm in tourmaline, corresponding to only 0.0087 wt% BeO.

The resulting empirical composition of the RK tourmaline is:



The GR tourmaline composition is:



Based on these compositions, stoichiometric calculations give 27.25 O atoms for RK and 27.08 O atoms for GR. These are close to the theoretical value of 27 O a.p.f.u. in tourmaline, excluding the V and W sites. Both tourmalines classify as **fluor-schorl** (Ertl *et al.* 2016). The RK sample has minor (fluor-)dravite and (fluor-)elbaite components. Sample GR is characterised by a distinct (fluor-)elbaite component and also more elevated Mn contents. The high standard deviation for FeO in sample GR (Table 2) is a corollary of the weak zonation observed in BSE images (see above).

The results of the crystal-structure refinements of two representative fragments of RK and GR are in good agreement with the chemical-analytical data. Selected bond lengths and the final refined formulae are provided in Table 3. For sample RK, the initial free refinement gave the simplified formula

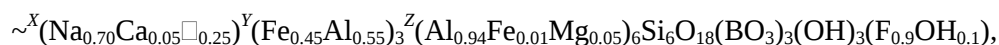


with ^YFe and ^YAl including any Li, Mg, Mn and Ti contents. The $\langle Y\text{-O} \rangle$ bond length indicated Li not more than 0.1 a.p.f.u. and only minor Mg on the Y site. The $X\text{-O}_2$ bond length suggested very minor or no Ca on the X site. The $\langle T\text{-O} \rangle$ value indicated only (very) minor Al on the T site, if any, and no excess B. The simplified formula compares well with the independently established EPMA-derived formula (based on 6 Si atoms):



In the final refinement step, the X- and Y-site occupancies were fixed to those of the EPMA-derived formula (Table 3). Since there was no chemical-analytical evidence for vacancies on the Y site, its occupancy was fixed to 3.00 a.p.f.u., and excess Fe was assigned as Fe^{3+} to the Z site, in agreement with the refined Z-site occupancy, $\text{Al}_{0.98}\text{Fe}_{0.02}$, and $\langle Z\text{-O} \rangle$ of 1.917 Å (*cf.* Ertl *et al.* 2012; Bačík 2015). The $R1(F)$ value was unchanged at 1.81%, attesting to the correctness of the bulk chemical composition.

For sample GR, the initial free refinement gave the simplified formula



with ^YFe and ^YAl again including any Li, Mg, Mn and Ti contents. The $\langle Y\text{--O} \rangle$, $X\text{--O}_2$, $\langle Z\text{--O} \rangle$, and $\langle T\text{--O} \rangle$ bond lengths suggested similar occupancy features as in sample RK (see above), but with slightly higher Ca and Al contents and less Fe, but very minor Mg on Z. The simplified formula compares again well with the independently established EPMA-derived formula (based on 6 Si atoms):



However, the discrepancy between refined and measured F:OH is higher than in sample RK. In the final refinement step, the X- and Y-site occupancies were again fixed to those of the EPMA-derived formula (while fixing the Y-site occupancy to 3.00 a.p.f.u.), and only Fe^{3+} was allowed as a minor substituent on the Z site (Table 3). The $R1(F)$ value was only slightly increased by 0.04%.

The smaller unit-cell parameters of the GR sample are caused by the higher (Al+Li) and lower Fe contents on its Y site. The low bulk Li contents of both samples fit well the negative correlation between the unit-cell parameter a and Li content of members of the elbaite-schorl series (Ertl *et al.* 2010). The mean $T\text{--O}$ bond lengths are similar in both samples (1.622 Å for RK, 1.621 Å for GR; Table 3) and suggest only very minor Al, if any, on the T site. The mean $Z\text{--O}$ lengths (1.917 Å for RK, 1.914 Å for GR) are consistent with Z being filled completely with Al in GR and probably very minor additional Mg in RK. Occupancy refinements gave evidence for very minor Fe^{3+} on the Z site of both RK and GR, with refined occupancies of $^Z(\text{Al}_{0.973(2)}\text{Fe}_{0.027(3)})$ and $^Z(\text{Al}_{0.968(3)}\text{Fe}_{0.032(3)})$, respectively). The fairly long mean $Y\text{--O}$ bond length in sample RK (2.054 Å) is caused by higher Fe and Mg contents (*cf.* Table 2) compared to GR which has $\langle Y\text{--O} \rangle = 2.045$ Å. The $X\text{--O}_2$ bond lengths (Table 3) are very similar and reflect very minor Ca and K on the X site (Ertl *et al.* 2001).

The refined F:OH ratios on the W site for RK and GR [0.87(7):0.13(7) and 0.98(9):0.02(9), respectively (Table 3), with an estimated real error of 0.1–0.2 F a.p.f.u., *cf.* Ertl *et al.* (2016)], are in reasonably good agreement with the average ratios determined by EPMA (RK: $\text{F}_{0.61}\text{OH}_{0.39}$; GR: $\text{F}_{0.54}\text{OH}_{0.46}$). However, locally there will be a minor variation of the F content inside each sample, and a minor analytical error for the measured F contents can also be expected, as is pointed out at the beginning of this section. Furthermore, the grains studied by single-crystal X-ray diffraction were not characterised by EPMA. We point out that the $Y\text{--W}$ bond length of 2.0733(14) in RK and 2.0623(18) in GR predicts an F:OH ratio of about 0.75:0.15 and 0.65:0.35, respectively, according to the very recently established correlation between the refined F content and the $Y\text{--W}$ (F,OH) bond length (Ertl *et al.*, 2016). Both refined and predicted ratios are higher than those determined from the EPMA data.

Discussion

Interpretation of the two data sets is impeded by the fact that the samples were not collected *in situ*, but rather from the mine dumps. Observations of the internal structure of the Høydaalen pegmatites were made by Oftedal in the years 1940 to 1942 (Oftedal 1942), and extensive quarrying has taken place since that time. However, building on the early observations made by Oftedal (1942), the main parts of the two samples studied here (with coarse albite and quartz) most likely belong to the outer zones of the primary pegmatite. Sample RK additionally contains a small area with cleavelandite. The

brown tourmaline of this sample occurs in the albite/quartz part and must be assumed to belong to the primary pegmatite phase. Oftedal (1942) attributes beryl and micas (muscovite and lepidolite) entirely to the cleavelandite phase. The green tourmaline of sample GR, embedded in beryl and muscovite that occur along small-scale shear zones cutting coarse albite/quartz, should accordingly be referred to the cleavelandite phase. As cleavelandite is absent in the sample, this may not necessarily be so. The tourmaline growth could be associated with some late event that pre- or postdates the main cleavelandite phase.

Tourmaline of the RK sample is higher in Fe, Mg and Ti compared to tourmaline in GR, while the GR tourmaline is higher in Li, Al and Mn relative to RK tourmaline. These relatively small but significant differences in geochemical signatures are considered to be consistent with the interpretations made above: RK tourmaline was formed in the early (primary) phase of pegmatite formation, whereas GR tourmaline belongs to a later (secondary) phase.

The scarcity of tourmaline and other boron minerals in the Høydalen pegmatites clearly indicates a very limited concentration of boron in the pegmatitic fluids. The only other boron mineral reported from the Høydalen pegmatites is an axinite-group mineral occasionally occurring at the border zone to the country rock (Raade *et al.* 1993). Oftedal (1964) has reported 0.03–0.1 wt% B₂O₃ in late-formed pink muscovite from Høydalen.

A crucial question is why there is no Li-rich tourmaline (elbaite) in the Høydalen area. Based on the considerations made above, the main cleavelandite phase must have been virtually devoid of boron, and the major part of lithium was consumed in the formation of lepidolite. In other areas, lepidolite-subtype pegmatites may be rich in tourmaline. Selway *et al.* (1999) studied the compositional evolution of tourmaline in five symmetrically zoned lepidolite pegmatites in the Czech Republic. From the outer to the inner zones, tourmaline compositions varied from foitite [${}^X\Box{}^Y(\text{Fe}^{2+}_2\text{Al})$] to schorl [${}^X\text{Na}^Y\text{Fe}^{2+}_3$], to elbaite [${}^X\text{Na}^Y(\text{Li}_{1.5}\text{Al}_{1.5})$] and rossmanite [${}^X\Box{}^Y(\text{LiAl}_2)$].

Acknowledgements

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Table 1. Crystal data, data collection information and refinement details for Høydalen fluor-schorl samples RK and GR.

Sample	RK	GR
a, c (Å)	15.987(2), 7.163(1)	15.967(2), 7.147(1)
V (Å ³)	1585.5(4)	1578.0(4)
Collection mode, $2\theta_{\max}$ (°)	full sphere, 75.56	full sphere, 75.54
h, k, l ranges	-27/27, -23/23, -12/12	-27/27, -23/23, -12/12
Total reflections measured	3744	3719
Unique reflections	2031 (R_{int} 1.16%)	2019 (R_{int} 1.04%)
$R1(F)$, $wR2_{\text{all}}(F^2)$	1.81%, 4.67%	2.08%, 5.49%
Flack x parameter	0.020(12)	0.012(15)
'Observed' refls. [$F_o > 4\sigma(F_o)$]	2006	1990
Extinct. coefficient	0.00273(18)	0.00051(16)
No. of refined parameters	98	96
GooF	1.143	1.129
$(\Delta/\sigma)_{\max}$	0.001	0.000
$\Delta\sigma_{\min}$, $\Delta\sigma_{\max}$ (e/Å ³)	-0.84, 0.85	-1.02, 1.24

Notes: Diffractometer: Nonius KappaCCD system; space group $R3m$; refinement on F^2 .

Table 2. Chemical composition of two fluor-schorl samples from Høydalen, Tørdal.

Sample RK					Sample GR				
Weight % oxide	SD	Atoms on Si = 6			Weight % oxide	SD	Atoms on Si = 6		
Li ₂ O	0.19		Li	0.13	Li ₂ O	0.47		Li	0.32
Na ₂ O	2.43	0.04	Na	0.80	Na ₂ O	2.15	0.11	Na	0.70
K ₂ O	0.04	0.01	K	0.01	K ₂ O	0.02	0.01	K	0.004
MgO	2.02	0.08	Mg	0.51	MgO	0.17	0.03	Mg	0.04
CaO	0.13	0.04	Ca	0.02	CaO	0.08	0.02	Ca	0.01
MnO	0.53	0.05	Mn	0.08	MnO	1.12	0.20	Mn	0.16
FeO	12.73	0.22	Fe ²⁺	1.80	FeO	11.38	0.73	Fe ²⁺	1.59
B ₂ O ₃ *	10.29*		B	3.00	B ₂ O ₃ *	10.42*		B	3.00
Al ₂ O ₃	32.56	0.31	Al	6.47	Al ₂ O ₃	34.69	0.43	Al	6.82
SiO ₂	35.56	0.15	Si	6.00	SiO ₂	35.96	0.47	Si	6.00
TiO ₂	0.66	0.10	Ti	0.08	TiO ₂	0.16	0.06	Ti	0.02
H ₂ O**	3.01**		H	3.39	H ₂ O**	3.11**		H	3.46
F	1.15	0.14	F	0.61	F	1.02	0.17	F	0.54
O=F ₂	-0.48				O=F ₂	-0.43			
Sum	100.82				Sum	100.32			

SD = standard deviation.

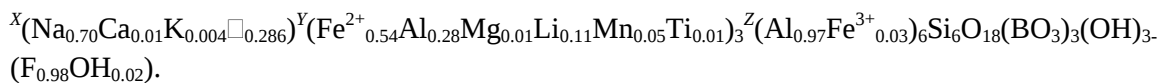
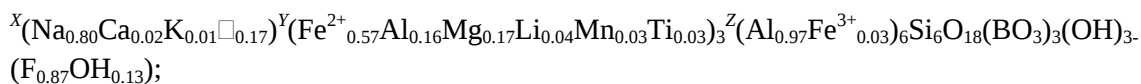
* Calculated to give B = 3 a.p.f.u.

** Calculated to give OH + F = 4 a.p.f.u.

Table 3. Selected interatomic distances ($\text{\AA}$) in Høydalen fluor-schorl samples RK and GR.

	RK	GR		RK	GR
X–O2 (x3)	2.4966(19)	2.487(2)	Y–O2 (x2)	2.0019(8)	1.9852(10)
–O5 (x3)	2.7635(14)	2.7751(17)	–O6 (x2)	2.0448(8)	2.0417(10)
–O4 (x3)	2.8207(14)	2.8292(18)	–W (F)	2.0733(14)	2.0623(18)
<X–O>	2.694	2.697	–O3	2.1602(13)	2.1546(16)
			<Y–O>	2.054	2.045
Z–O6	1.8647(8)	1.8600(10)	T–O6	1.6063(8)	1.6069(9)
–O7	1.8842(8)	1.8804(9)	–O7	1.6139(8)	1.6149(9)
–O8	1.8868(8)	1.8844(9)	–O4	1.6267(5)	1.6254(5)
–O8	1.9247(8)	1.9215(10)	–O5	1.6403(5)	1.6379(6)
–O7	1.9634(8)	1.9616(10)	<T–O>	1.622	1.621
–O3	1.9777(6)	1.9737(7)			
<Z–O>	1.917	1.914			
			Hydrogen bonds		
B–O2	1.3628(19)	1.360(2)	O3–H	0.89(4)	0.84(4)
–O8 (x2)	1.3846(11)	1.3857(13)	O3···O5	3.2195(16)	3.1996(19)
<B–O>	1.377	1.377	O3–H···O5	158(3) $^\circ$	157(4) $^\circ$

The final refined formulae for RK and GR are, respectively:



The X- and Y-site occupancies were fixed to those of the EPMA-derived formulae. The probably very minor Mg-for-Al substitution on the Z site in both tourmalines has been neglected.