

Chemical composition and crystal structure refinement of schorl from the Lundazi pegmatite field, Zambia

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Abstract. Present work characterizes tourmaline from one of the major pegmatite fields in Zambia – the Lundazi pegmatite belt.

Microprobe analysis gave (wt%): SiO₂ 34.65, TiO₂ 0.85, Al₂O₃ 29.80, Fe₂O₃ 4.94, FeO 9.47, MnO 0.29, MgO 4.06, Li₂O < 0.01, CaO 0.59, Na₂O 2.38, K₂O 0.08, F 0.32, H₂O+ 3.24, B₂O₃ 10.32, O=F -0.14, totalling 100.45. The empirical formula, calculated on the basis of 31 (O, OH, F) per formula unit gives: (Na_{0.78}Ca_{0.11}K_{0.02}F_{0.09})_{Σ1.00}(Fe²⁺_{1.33}Fe³⁺_{0.63}Mg_{0.61}Ti_{0.11}Mn_{0.04})_{Σ2.00}(Al_{5.59}Mg²⁺_{0.41})_{Σ6.00}[(Si_{5.84}Al_{0.16})_{Σ26.00}O_{18.00}]_{Σ1.00}(BO₃)_{3.00}[(OH)_{0.64}O_{0.19}F_{0.17})_{Σ1.00} resulting in simplified formula: Na(Fe²⁺,Fe³⁺,Mg)₃(Al,Mg)₆(Si₆O₁₈)(BO₃)₃(OH,O,F). Analysis of Mössbauer spectra confirms both Fe²⁺ and Fe³⁺ in the Y site; Fe³⁺/Fe²⁺ is 0.47. The water was determinate using Karl Fischer titration, B₂O₃ was calculated to stoichiometry. Refined crystal structure data (atomic coordinates, inter-atomic distances and angles) are in agreement with data for schorl. Mean polyhedron distances are (Å): X-O 2.646, Y-O 2.078, Z-O 1.939, Si-O 1.644, B1-O 1.382. The refined unit-cell parameters are: *a* = 15.9856 (2), *c* = 7.1892 (1) Å, *V* = 1591.00(4) Å³, space group is *R*3*m*, *Z*=3, *D*_m = 3.18(1) g/cm³, *D*_x = 3.195(2) g/cm³. Streak is light grey, lustre is glassy. Pleochroism in powder mounts: ε = light brownish red, ω = dark bluish grey (thin fragments), ε = strong brownish red, ω = opaque (thick fragments). The studied sample belongs to hydroxy-tourmaline subgroup with 19 atomic % of oxy subgroup (Fe³⁺/Fe²⁺ = 0.47 in the Y site and ratio O/(OH⁻) = 0.30 in the W site).

Abstract. Práce charakterizuje turmalín z jedné z hlavních pegmatitových lokalit Zambie – pegmatitového pásmo Lundazi.

Lokální bodová analýza (LAREM) poskytla chemickou analýzu (hm.%): SiO₂ 34.65, TiO₂ 0.85, Al₂O₃ 29.80, Fe₂O₃ 4.94, FeO 9.47, MnO 0.29, MgO 4.06, Li₂O < 0.01, CaO 0.59, Na₂O 2.38, K₂O 0.08, F 0.32, H₂O+ 3.24, B₂O₃ 10.32, O=F -0.14, suma 100.45. Empirický vzorec rozpočtený na 31 (O, OH, F) atomů na vzorcovou jednotku poskytuje: (Na_{0.78}Ca_{0.11}K_{0.02}F_{0.09})_{Σ1.00}(Fe²⁺_{1.33}Fe³⁺_{0.63}Mg_{0.61}Ti_{0.11}Mn_{0.04})_{Σ2.00}(Al_{5.59}Mg²⁺_{0.41})_{Σ6.00}[(Si_{5.84}Al_{0.16})_{Σ26.00}O_{18.00}]_{Σ1.00}(BO₃)_{3.00}[(OH)_{0.64}O_{0.19}F_{0.17})_{Σ1.00}, zjednodušeně: Na(Fe²⁺,Fe³⁺,Mg)₃(Al,Mg)₆(Si₆O₁₈)(BO₃)₃(OH,O,F). Analýza Mössbauerova spektra potvrdila Fe²⁺ a Fe³⁺ pouze v pozicích Y; vypočtený poměr Fe³⁺/Fe²⁺ je 0.47. Voda byla stanovena Karl Fischerovou titrací, B₂O₃ byl dopočten ze stechiometrie. Zpřesněná data krystalové struktury (pozice atomů, meziatomové vzdálenosti a úhly) jsou v dobré shodě s daty pro skoryl. Střední vzdálenosti polyedrů jsou (Å): X-O 2.646, Y-O 2.078, Z-O 1.939, Si-O 1.644, B1-O 1.382. Zpřesněné parametry základní celly jsou: *a* = 15.9856 (2), *c* = 7.1892 (1) Å, *V* = 1591.00(4) Å³, s.g. *R*3*m*, *Z* = 3, *D*_m = 3.18(1) g/cm³, *D*_x = 3.195(2) g/cm³. Vryp je světle šedý, lom skelný. Pleochroismus práškového preparátu: ε = světle hnědavě červená, ω = tmavě modravě šedá (tenké fragmenty), ε = silně hnědavě červená, ω = opakní (silné fragmenty). Studovaný vzorek patří do podskupiny hydroxy turmalínů s 19 atom. % oxy složky.

Key words: pegmatite, tourmaline, schorl, chemical composition, crystal structure, refinement, cell parameters, pleochroism, Mössbauer spectroscopy, XRD powder diffraction

Introduction

During the last two decades, Zambia became an important producer of gem-quality tourmalines (Milisenda et al. 2000). One of the major pegmatite fields in this country is the Lundazi pegmatite belt. This area also produced a unique, greenish-yellow gem-quality elbaitic tourmaline with MnO contents ~ 6–8 wt% (Thomas 1982, Schmetzer and Bank 1984, Shigley et al. 1986, Nuber and Schmetzer 1984). In the recently proposed tourmaline classification (Hawthorne and Henry 1999), this Mn-rich tourmaline from Zambia is classified as a member nearly halfway between oxy-elbaite and oxy-manganofoitite. Crystallisation of pegmatitic tourmaline with such composition suggests unusual conditions of mineralization.

Except for some data on gem-quality tourmalines and aquamarine, detailed mineralogical information on pegmatites in the Lundazi belt is lacking. In this con-

text, we considered the mineralogical characterisation of schorl tourmaline from an ordinary tourmaline pegmatite in this area as an interesting contribution to knowledge of local pegmatite mineralization.

Deposit characteristics

One of the major pegmatite fields in Zambia is the Lundazi pegmatite belt, extending at a distance of 200 km southwest of Lundazi in the Eastern Province (Fig. 1). A simple tourmaline pegmatite is exposed on the western side of the main road from Lundazi to Chama, 3 km north of Lundazi, opposite the Tigone Basic School. The exposed part includes 5–8 m wide quartz core, with predominant pink quartz and parts of the block pegmatite zone with 60 cm long crystals of K-feldspar, white quartz and some fractured pieces to 4 cm wide of black schorl tourmaline (sample LZ-2). Rare

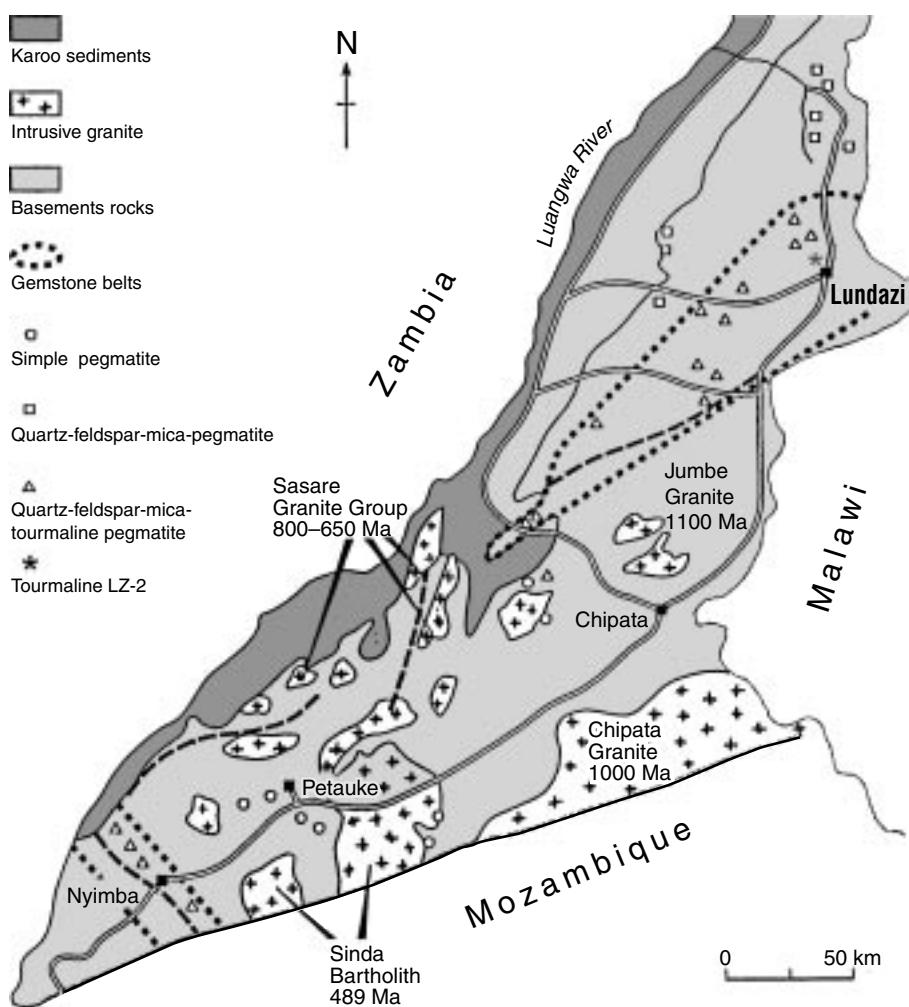


Fig. 1. Pegmatite localities and granite intrusions in part of eastern Zambia, following Watts et al. (1991), simplified.

fragments of manganese ilmenite (5.4 wt% MnO) to 3 cm long have been found in the loose material.

During the brief visit, no information was obtained on possible relations of this pegmatite to granites in the wider area. Imperfect exposure, confined to quartz-rich core of the dyke, prevented sampling and characterization of other parts of the dyke.

Physical and optical properties

Streak of Lundazi schorl is light grey, lustre is glassy. The density of crystal fragments measured by double weighing method is $3.18(1) \text{ g/cm}^3$ and the calculated crystal density (for $Z = 3$) is $3.195(2) \text{ g/cm}^3$.

Schorl is optically negative. Pleochroism in powder mounts: ϵ = light brownish red, ω = dark bluish grey (thin fragments), ϵ = strong brownish red, ω = opaque (thick fragments).

Analytical methods – sample preparation

To remove minor limonitic staining, sample used for X-ray powder diffraction, H_2O determination, Mössbauer spectra measurements, and atomic absorption analysis was purified in 5% HCl, followed by repeated bath in distilled H_2O . All the data and microprobe analyses have been obtained on material from the same crystal.

The qualitative and quantitative chemical composition was measured with a scanning electron microprobe CamScan 4 with an energy-dispersive analyser LINK eXL and a wave-dispersive analyser Microspec WDX-3PC. The following conditions were used: operating voltage 15 kV, sample current 3 nA, specimen beam size 1(1 μm , and simple synthetic compounds as standards. Correction procedure Phi(rho(Z)) was used for calculation of all quantitative analyses. The $\text{Fe}^{3+}/\text{Fe}^{2+}$

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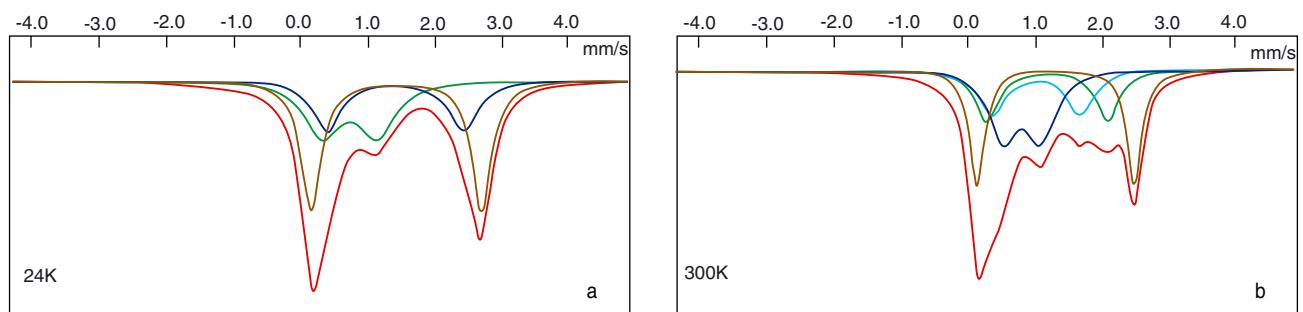


Fig. 2. a – Mössbauer spectra of Lundazi schorl at 300K; b – Mössbauer spectra of Lundazi schorl at 24K.

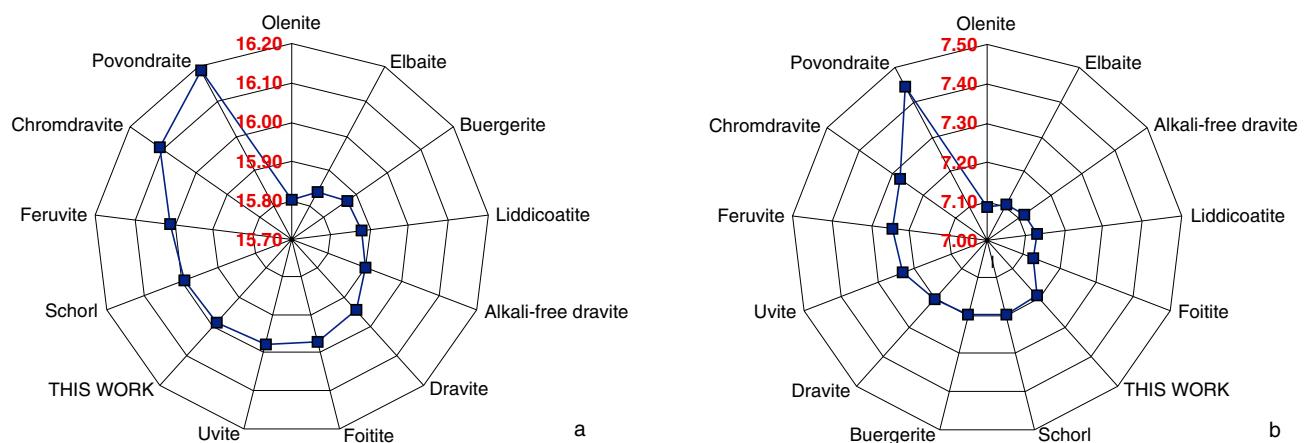


Fig. 3. a – Comparison of unit cell parameter a (Å) of Lundazi schorl and other common tourmalines; b – Comparison of unit cell parameter c (Å) of Lundazi schorl and other common tourmalines.

ratio was determined by Mössbauer spectra, water was measured using Karl Fischer titration. The content of B_2O_3 was calculated to stoichiometry. Fluorine was analysed by ISE, Li by atomic absorption.

Powder diffraction data were collected using a Philips X'Pert MPD diffractometer equipped with a sealed copper tube and a graphite secondary monochromator. High voltage was set to 40 kV and tube current to 40 mA. Powder pattern was collected in the range from 15 to 130 $^{\circ}2\theta$ CuK_{α} with step size of 0.02 $^{\circ}2\theta$ CuK_{α} and exposure of 12 sec. per a step. To minimize complicated shape of background due to classic glass sample holders, the sample studied was placed atop a flat silicon wafer from alcoholic suspension.

Chemical composition

The quantitative chemical composition (Table 1) of Lundazi schorl was determined from seven spot analyses showing minimal variation.

The following minor and trace elements were determined by atomic absorption (ppm): 12 Be, 49 Cr, 8 Co, 418 Zn, 15 Cu, 11 Rb, 22 Ni, 22 Sr, 120 V, 58 Ba, 44 Pb, 8 Mo.

Mössbauer spectra were measured at the temperature 24 and 300K (Figs 2a,b). Three doublets were used to approximate observed spectrum at 24K. Two doublets (δ in mm/s, Δ in mm/s, Area in %) 1.403(6), 2.03(2), 24(1) and 1.419(1), 2.536(3), 44(1) correspond to $^{[Y1]}\text{Fe}^{2+}$, and $^{[Y2]}\text{Fe}^{2+}$ respectively (Dyar et al. 1998). Doublet at 0.713(7), 0.81(1), 31.8(2) corresponds to $^{[Y]}\text{Fe}^{3+}$. Analysis of Mössbauer spec-

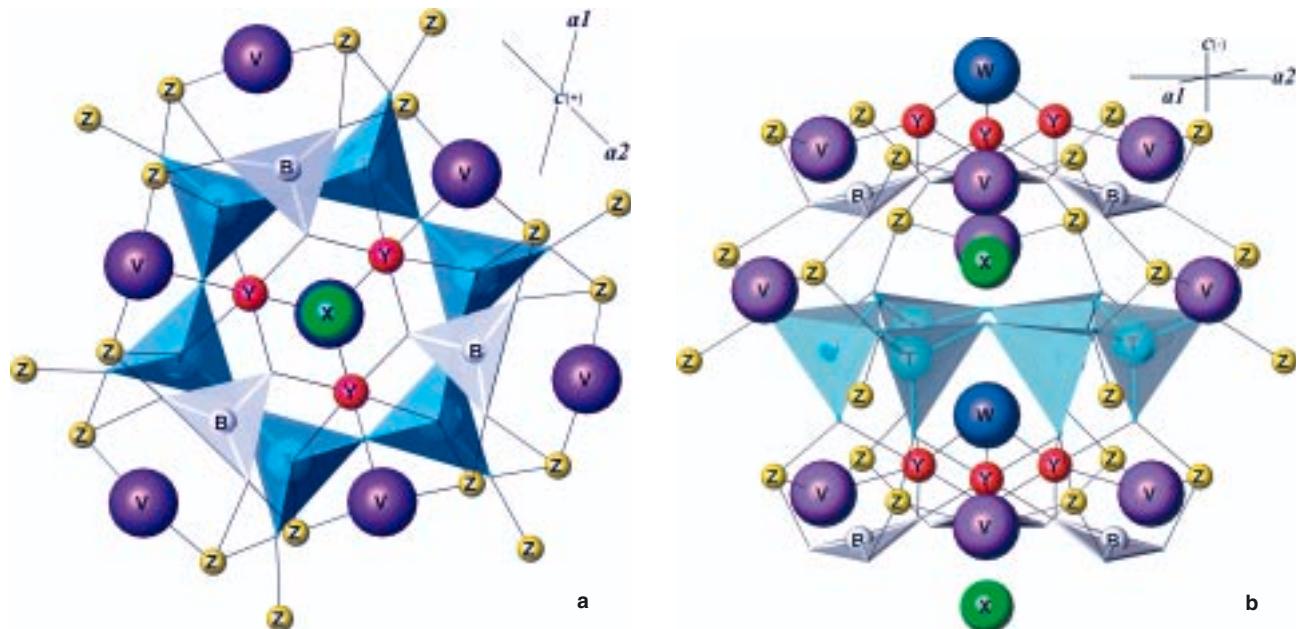


Fig. 4. a – Projection of tourmaline crystal structure onto the 001 plane; b – Projection of tourmaline crystal structure onto the slightly sloping 100 plane.

Table 1. Chemical composition of schorl from Lundazi.

	wt %	number of atoms #	
SiO ₂	34.65	Si	5.835
TiO ₂	0.85	Ti	0.108
Al ₂ O ₃	29.80	Al	5.915
Fe ₂ O ₃ *	4.94	Fe ³⁺	0.626
FeO*	9.47	Fe ²⁺	1.334
MnO	0.29	Mn	0.041
MgO	4.06	Mg	1.019
Li ₂ O	< 0.01	Li	0.000
CaO	0.59	Ca	0.106
Na ₂ O	2.38	Na	0.777
K ₂ O	0.08	K	0.017
F	0.32	F	0.170
H ₂ O ⁺ *	3.24	H	3.640
B ₂ O ₃ **	10.32	B	3.000
O=F	-0.14	O	30.830
Total	100.45		

* Fe³⁺/Fe²⁺ ratio = 0.47 indicated by Mössbauer spectra; ** B₂O₃ calculated to stoichiometry; * direct determination by Karl Fischer titration; # atoms per formula unit (apfu) on the basis of 31 (O, OH, F) per formula unit

tra at 300K confirms both Fe²⁺ and Fe³⁺ valence in the Y octahedral site; the ratio of Fe³⁺/Fe²⁺ is 0.47(5).

Table 2. Recalculation of chemical analysis of Lundazi schorl according to structural formula XY₃Z₆(T₆O₁₈)(BO₃)₃V₃W.

	X	Y	Z	T	(BO ₃)	V3	W
vacancy	0.10	0.12					
Si					5.84		
Ti		0.11					
Al		0.16	5.59	0.16			
Fe ³⁺		0.63					
Fe ²⁺		1.33					
Mn		0.04					
Mg		0.61	0.41				
Ca	0.11						
Na	0.78						
K	0.02						
BO ₃					3.00		
F							0.17
OH						3.00	0.64
O							0.19
Sum	1.00	3.00	6.00	6.00	3.00	3.00	1.00

Microprobe spot analyses across a 2 cm long section of tourmaline and optical observation under the microscope indicate a notable compositional homogeneity of this tourmaline and the absence of inclusions.

Table 3. X-ray powder diffraction pattern of Lundazi schorl from the Rietveld refinement.

I _{rel}	d	h	k	l	I _{rel}	d	h	k	l	I _{rel}	d	h	k	l
76	6.380	1	0	1	3	1.8337	7	1	0	3	1.4225	1	9	1
33	4.986	0	2	1	4	1.8204	6	1	2	28	1.4105	4	3	4
22	4.615	3	0	0	19	1.7823	1	0	4		1.4102	6	3	3
66	4.231	2	1	1		1.7817	3	3	3		1.4102	3	6	3
59	3.996	2	2	0	2	1.7442	6	3	0	4	1.4078	2	0	5
100	3.479	0	1	2	15	1.7396	0	2	4	2	1.3864	1	2	5
13	3.387	1	3	1		1.7328	0	7	2	3	1.3795	3	8	1
8	3.190	2	0	2		1.7328	5	3	2	2	1.3685	1	6	4
19	3.021	4	1	0	2	1.7210	5	4	1	13	1.3594	10	0	1
97	2.9628	1	2	2	12	1.6934	2	6	2	9	1.3465	3	1	5
16	2.9052	3	2	1	38	1.6621	0	6	3		1.3457	5	6	2
15	2.6241	3	1	2		1.6621	6	0	3		1.3457	9	1	2
84	2.5838	0	5	1	18	1.6464	2	7	1	15	1.3321	6	6	0
10	2.4932	0	4	2	4	1.6273	5	2	3		1.3301	3	5	4
10	2.4585	2	4	1		1.6273	2	5	3		1.3301	7	0	4
28	2.3964	0	0	3	31	1.5986	5	5	0	13	1.3298	5	5	3
28	2.3801	2	3	2		1.5950	4	0	4		1.3278	0	4	5
20	2.3499	5	1	1	4	1.5898	4	5	2	17	1.3140	10	1	0
6	2.3073	6	0	0	3	1.5807	8	1	1		1.3121	6	2	4
4	2.2954	1	1	3	3	1.5642	3	2	4	4	1.3099	2	3	5
7	2.2168	5	2	0	7	1.5506	4	6	1	5	1.3091	8	3	2
24	2.1935	5	0	2	6	1.5382	9	0	0	4	1.3040	5	7	1
18	2.1698	4	3	1	8	1.5304	7	2	2	3	1.2945	9	0	3
34	2.1267	3	0	3	2	1.5223	7	3	1	2	1.2919	0	10	2
	2.1267	0	3	3	2	1.5105	8	2	0	3	1.2870	8	4	1
12	2.1153	4	2	2	37	1.5075	0	5	4	5	1.2799	9	3	0
30	2.0552	2	2	3	10	1.4814	2	4	4	5	1.2778	2	8	3
58	2.0449	1	5	2	5	1.4772	1	8	2	26	1.2760	5	0	5
18	2.0256	1	6	1	53	1.4566	5	1	4	7	1.2620	5	4	4
8	1.9982	4	4	0		1.4563	7	1	3	3	1.2441	7	5	2
41	1.9229	3	4	2		1.4563	1	7	3	7	1.2397	0	11	1
4	1.9069	7	0	1		1.4526	6	4	2	4	1.2315	4	7	3
23	1.8774	1	4	3	9	1.4356	7	4	0	3	1.2293	4	8	2
	1.8774	4	1	3	16	1.4301	0	1	5	3	1.2250	2	10	1
12	1.8548	6	2	1	10	1.4225	6	5	1	6	1.2156	3	4	5

h, k, l indexing on the basis of the crystal structure data (Grice et al. 1993), observed integral intensities ($I_{\text{rel}} > 2$) in % scale.

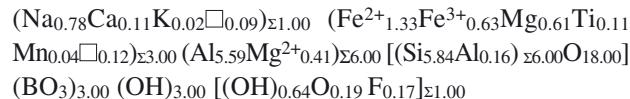
Table 4. Conditions and results of the Rietveld crystal structure refinement of Lundazi schorl.

Formula:	$(Na_{0.78}Ca_{0.14}\square_{0.09})(Fe_{2.30}Mg_{0.70})_3(Al_{5.59}Mg_{0.41})_6(Si_6O_{18})(BO_3)_3(OH)_3O$		
Diffractometer: Philips X'Pert System MPD			
Wavelengths, $\lambda(\text{\AA})$	1.5405 + 1.5443	$V(\text{\AA}^3)$	1591.00(4)
2θ range ($^{\circ}2\theta$)	15-130	Z	3
Step width ($^{\circ}2\theta$)	0.02	$D_x(\text{g.cm}^{-3})$	3.195(2)
Counting time (sec.)	10	overall temp. factor (\AA^2)	0.100
No. of observations	5751	R_p (%)	6.69
No. of reflections	705	R_{wp} (%)	8.55
No. of fitted variables	36	R_{exp} (%)	9.82
Space group	$R3m$	R_B (%)	15.3
Unit cell parameters:		R_F (%)	10.5
$a(\text{\AA})$	15.9856(2)	χ^2	0.757
$c(\text{\AA})$	7.1892(1)	Convergence criterion, ϵ	0.10

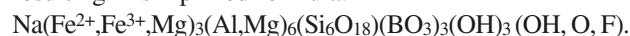
The empirical formula of schorl from Lundazi was calculated according to following presumptions:

1. ratio of Fe^{3+}/Fe^{2+} is 0.47 this work
2. $[Z]Mg = (2.086 - [Y]Fe^{2+})/1.84$ (Blooddaxe et al., 1999)
3. Ti is assigned to the Y site (Hawthorne et al., 1993) basis of structural formula is $XY_3Z_6(T_6O_{18})(BO_3)_3V_3W$ (Hawthorne – Henry, 1999)
4. composition is normalized to 31 (O, OH, F) per formula unit (Deer et al., 1992)
5. no vacancies are expected on the T and Z sites

so that the recalculated formula (see Table 2) gives:



resulting in simplified formula:



The recalculation of molar ratios of Fe^{2+} , Fe^{3+} , Mg and Al in crystallographic sites Y, Z was verified from three probable possibilities:

Y	Z
1. $Fe^{2+}_{1.33}Fe^{3+}_{0.63}Mg_{0.61}Ti_{0.11}Mn_{0.04}\square_{0.12}$	$Al_{5.59}Mg^{2+}_{0.41}$
2. $Fe^{2+}_{1.33}Mg_{1.02}Fe^{3+}_{0.54}Mn_{0.04}$	$Al_{5.91}Fe^{3+}_{0.09}$
3. $Fe^{2+}_{1.33}Mg_{1.02}Al_{0.54}Mn_{0.04}$	$Al_{5.37}Fe^{3+}_{0.63}$

Table 5. Atomic coordinates of schorl from Lundazi (with e. s. d.'s in parentheses) from the Rietveld crystal structure refinement.

Atom	x	y	z
X	0	0	0.2363(22)
Y	0.1177(4)	2x	0.6376(7)
Z	0.2926(4)	0.2603(4)	0.6071(8)
B1	0.1395(20)	2x	0.9885(32)
Si1	0.1905(4)	0.1926(4)	0
O1	0	0	0.7923(32)
O2	0.0592(11)	2x	0.5010(18)
O3	0.2834(12)	1/2x	0.5322(20)
O4	0.0918(12)	2x	0.0616(19)
O5	0.1887(12)	1/2x	0.1042(22)
O6	0.1923(9)	0.1909(8)	0.7753(11)
O7	0.2902(7)	0.2840(8)	0.0875(16)
O8	0.2030(7)	0.2554(7)	0.4155(14)

Occupation in sites: X = $Na_{0.78}Ca_{0.14}\square_{0.09}$; Y = $Fe_{2.30}Mg_{0.70}$;

Z = $Al_{5.59}Mg_{0.41}$; Si1 = $Si_{6.00}$

Table 6. Selected bond lengths (Å) of schorl from Lundazi.

X	O2 $\times 3$	2.513(18)	Z	O7'	1.961(12)
X	O5 $\times 3$	2.780(19)	Z	O8	1.960(13)
Y	O1	2.067(15)	Z	O8'	2.029(14)
Y	O2 $\times 2$	1.908(17)	Si1	O4	1.575(21)
Y	O3	2.417(21)	Si1	O5	1.728(19)
Y	O6 $\times 2$	2.083(13)	Si1	O6	1.616(8)
Z	O3	1.904(18)	Si1	O7	1.655(13)
Z	O6	1.867(13)	B1	O2	1.631(34)
Z	O7	1.910(13)	B1	O8 $\times 2$	1.257(41)
Mean polyhedron distance					
X	O	2.646			
Y	O	2.078			
Z	O	1.939			
Si	O	1.644			
B1	O	1.382			

The crystal structure data were refined for each option and the fit parameters R_{wp} , R_p , χ^2 were compared. The results clearly show that the first option, used in the structural formula above, is the best solution.

X-ray powder diffraction and crystal structure refinement

X-ray powder diffraction pattern (Table 3) was indexed on the basis of the refined crystal structure data (Grice et al. 1993). Peak positions, intensities, refined atomic coordinates, inter-atomic distances and angles were calculated by program FullProf (Rodriguez-Carvajal 1998) using the Rietveld method (Table 4).

The refined unit-cell parameters are: $a = 15.9856$ (2), $c = 7.1892$ (1) Å, $V = 1591.00(4)$ Å 3 , space group is $R3m$, $Z=3$. The Figures 3a, b graphically compare a and c parameters with parameters for other common tourmalines.

Two projections of crystal structure of tourmaline are shown in Figures 4a and 4b. There are 31 anions in the structure formula that are located in 8 distinct sites O1

Table 7. Selected inter-atomic angles (°) of schorl from Lundazi.

O2 - X - O2	68.93(9)	O6 - Z - O8	92.19(8)
O2 - X - O5	150.77(11)	O6 - Z - O8	103.09(10)'
O2 - X - O5'	87.22(9)	O7 - Z - O7	89.33(9)
O5 - X - O5	108.97(11)	O7 - Z - O8	80.00(9)
O1 - Y - O2	88.97(12)	O7 - Z - O8	84.93(8)'
O1 - Y - O3	160.27(13)	O7 - Z - O8	105.69(9)''
O1 - Y - O6	95.67(8)	O7 - Z - O8	77.14(8)'''
O2 - Y - O2	96.40(13)	O8 - Z - O8	164.60(11)
O2 - Y - O3	104.00(13)	O4 - Si1 - O5	103.50(19)
O2 - Y - O6	84.98(10)	O4 - Si1 - O6	107.80(14)
O2 - Y - O6'	175.19(12)	O4 - Si1 - O7	116.87(17)
O2 - Y - O6''	84.99(10)	O5 - Si1 - O6	114.31(13)
O3 - Y - O6	71.20(8)	O5 - Si1 - O7	102.08(13)
O6 - Y - O6	93.27(9)	O6 - Si1 - O7	112.10(10)
O3 - Z - O6	88.60(12)	O2 - B1 - O3	160.07(18)
O3 - Z - O7	96.82(11)	O2 - B1 - O4	94.43(16)
O3 - Z - O7'	160.01(14)	O2 - B1 - O8	106.67(26)
O3 - Z - O8	94.12(12)	O3 - B1 - O4	65.65(11)
O3 - Z - O8'	84.45(10)	O3 - B1 - O8	74.50(22)
O6 - Z - O7	170.77(11)	O4 - B1 - O8	89.10(22)
O6 - Z - O7'	88.05(8)	O8 - B1 - O8	146.66(31)

through O8. The O2 and O4-O8 are occupied exclusively by O²⁻. The single O1 site, termed the W site in the structural formula, is located along the three-fold axis central to the pseudo-hexagonal ring of tetrahedra and contains: (OH)_{0.64}O_{0.36}F_{0.17}. The three O3 sites, termed the V site, contain for presented tourmaline OH groups only.

Apical oxygens of six-membered tetrahedral rings of TO₄ (T sites), characteristic for the tourmaline structure, point toward the c-pole. The T site occupation used with structure refinement is Si_{5.84}Al_{0.16}. The X site is a nine-coordinated trigonal antiprism, located along the three-fold axis of symmetry. For Rietveld refinement was used X = Na_{0.78}Ca_{0.14}.

The Y site is a relatively regular octahedral polyhedron occupied by Fe and Mg in proportion 1.96/0.61. The Z octahedron is relatively small, somewhat distorted, and occupied by Al and Mg in proportion 5.59/0.41.

The refined atomic coordinates and calculated interatomic distances and angles are presented in Tables 5, 6, and 7.

The statistical error ($R_{wp} = 8.55$) possibly indicates minor deviation of structure from perfectly ordered state. Alternatively, the error is due to compositional variation in the subsample measured.

Discussion

The crystallochemical formula indicates that the higher Fe³⁺ content in Lundazi schorl is due mainly to the following substitution in the Y site: Fe³⁺O Fe²⁺(OH)₋₁.

A comparison of the sample LZ-2 with a large set of analysed schorl tourmalines, e.g. Povondra (1981), shows that this tourmaline is not exceptional. It is near to composition of pegmatite schorl No. 84, from Ruprechtice, Krkonoše-Jizera granite pluton and another pegmatite schorl No. 57, from Bežerovice near Bechyně, Moldanubian Zone in south-central Bohemia. Common features of these tourmalines include somewhat lower SiO₂ and Al₂O₃ and higher Fe₂O₃, compared to ordinary schorl-dravite members with a similar Fe²⁺/Mg ratio.

Compared to the gem-quality Mn-rich elbaitic tourmaline from Mugwazo pegmatite, Lundazi pegmatite belt, the oxy tourmaline component in ferrous/ferric schorl LZ-2 is much lower but still attains appreciable values. Following the V and W sites occupancy scheme proposed by Hawthorne and Henry (1999), the schorl LZ-2 belongs to hydroxy subgroup of tourmalines with 19 atomic % of

oxy subgroup. The oxy-character is also expressed by the ratio Fe³⁺/Fe²⁺ = 0.47 in the Y site and ratio O/(OH⁻) = 0.30 in the W site.

The ferrous/ferric nature of the schorl studied indicates relatively high oxygen fugacity in the parent melt or a possible influence of accessory magnetite in the local metamorphic complex hosting the pegmatite.

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