

X-Ray and Optical Data for Alkali Cation-Deficient Schorls from Jack Creek, Montana, U.S.A. and Ben Lomond, North Queensland, Australia

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Abstract

X-ray powder diffraction and optical data are presented for alkali-deficient schorls from two tourmaline-dumortierite deposits. The compositions of both schorls reflect the presence of an alkali-defect substitution, whereby the alkali cation deficiencies in the crystal structure are charge balanced by trivalent for divalent cation substitutions in the octahedral sites. Refined unit cell and optical data are as follows: $a = 15.9523(15)$, $c = 7.1466(2)$ Å, $F_{30} = 104(0.009, 32)$, $M_{20} = 68$, $\epsilon = 1.638(2)$, $\omega = 1.660(2)$, $D_x = 3.12$ for the schorl from Jack Creek, near Basin, Montana, U.S.A. and $a = 15.9800(15)$, $c = 7.1504(2)$ Å, $F_{30} = 156(0.006, 32)$, $M_{20} = 152$, $\epsilon = 1.642(2)$, $\omega = 1.668(2)$, $D_x = 3.17$ for the schorl from Ben Lomond, Hervey Range, North Queensland, Australia. Indexed X-ray powder diffraction patterns are also presented.

Introduction

The tourmaline group has been long recognized for its extreme compositional variability. In addition to the substitutions relating the commonly recognized end-members schorl, $\text{NaFe}_3\text{Al}_6(\text{BO}_3)_3\text{Si}_6\text{O}_{18}(\text{OH})_4$, dravite $\text{NaMg}_3\text{Al}_6(\text{BO}_3)_3\text{Si}_6\text{O}_{18}(\text{OH})_4$ and elbaite $\text{Na}(\text{Li},\text{Al})_3\text{Al}_6(\text{BO}_3)_3\text{Si}_6\text{O}_{18}(\text{OH})_4$, many others have been revealed during detailed studies (Foit & Rosenberg, 1974, 1977; Rosenberg & Foit, 1986) of tourmalines from a wide variety of geologic environments. These substitutions produce a systematic variation in tourmaline structural parameters including unit cell parameters and cell volume (Foit, 1989), which explains why tourmaline powder diffraction patterns are often quite different.

Schorls from two tourmaline-dumortierite deposits (Jack Creek near Basin, Montana, U.S.A.; Ben Lomond, Hervey Range, North Queensland Australia) were chemically and structurally characterized to include microprobe and Mössbauer analysis, and crystal structure refinement (of Jack Creek schorl) during recent studies (Foit, 1989; Foit *et al.*, 1989). The powder X-ray data on these well-characterized tourmalines were not included in these reports and it is the purpose of this paper to make them available. The X-ray powder diffraction pattern of synthetic schorl (PDF 22-469) currently in the Powder Diffraction File appears to be incomplete, is only partially indexed and was collected to only $70^\circ 2\theta$. Its Smith/Snyder (1975) figure of merit (F_{25}) is 2 (0.134, 76).

Sample Preparation

Coverless thin sections, tourmaline separates and hand-picked tourmaline crystals were prepared from Jack Creek (JC3) and Ben Lomond (BL5) hand samples. After preparation of the thin sections to be used for electron microprobe analysis, the remainder of the hand sample was crushed to 60-200 mesh and a tourmaline concentrate was prepared by means of heavy liquid and isodynamic separation. The crystal used in the structure refinement (Foit, 1989) was also selected from the JC3 concentrate. Approximately 90 milligrams of tourmaline crystals of superior quality to be used in Mössbauer spectrographic analysis were hand-picked from

each of the concentrates. After the Mössbauer analysis was completed, the hand-picked crystals were ground to a grit-free consistency under ethanol and prepared for X-ray powder diffraction analysis.

Electron Microprobe and Optical Analysis

The experimental details for the electron microprobe analyses are given in Foit *et al.* (1989). The tourmaline chemical data presented in Table 1 represent a total of 56 point analyses on 37 BL5 schorl crystals and 72 analyses on 6 JC3 schorl crystals. These data are the means of the chemical data plotted on the scatter diagrams in Foit *et al.* (1989) and, therefore, are slightly different from the mean values for selected individual crystals given in Table 2 of that paper. The chemical zoning observed in the Jack Creek tourmalines necessitated the greater number of analyses per crystal. The chemical zoning is also reflected in the standard deviations of the oxide weight percents of Fe and Mg.

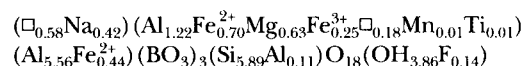
The Jack Creek and Ben Lomond tourmalines are uniaxial negative and display the strong pleochroism, $\epsilon = \text{col}$

Table 1.
Electron Microprobe Analyses

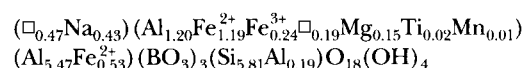
Oxide	Jack Creek		Ben Lomond	
	Wt%	Cations	Wt%	Cations
Na ₂ O	1.31(0.45)	0.42	1.34(0.19)	0.43
K ₂ O	0.02(0.02)	—	0.01(0.02)	—
CaO	0.01(0.01)	—	0.55(0.23)	0.10
MgO	2.58(2.02)	0.63	0.62(0.49)	0.15
MnO	0.04(0.05)	0.01	0.06(0.05)	0.01
FeO	8.34(2.14)*	1.14	12.41(0.69)	1.72
Fe ₂ O ₃	2.03(0.52)	0.25	1.88(0.08)	0.24
Al ₂ O ₃	35.77(0.99)	6.89	35.04(0.91)	6.86
B ₂ O ₃	10.62**	3.00	10.48	3.00
TiO ₂	0.06(0.06)	0.01	0.17(0.09)	0.02
SiO ₂	36.08(0.86)	5.89	34.98(0.80)	5.81
F	0.27(0.12)	0.14	n.d.	—
P	trace	—	n.d.	—
	97.13		97.54	
less O=F	-0.11			
H ₂ O	3.54**		3.61	
Total	100.56		101.15	

Formulae on the basis of 31 (O,OH,F):

Jack Creek



Ben Lomond



* Fe²⁺/Fe³⁺ proportions and site assignments determined by Mössbauer spectroscopy.

** Wt. % calculated assuming stoichiometric B₂O₃ and H₂O

orless, pale green and ω = green, bluish green, typical of most schorls. The refractive indices given in Table 2 were determined using white light and the Becki line oil immersion method (Bloss, 1961).

Table 2.
Unit Cell and Optical Data

	Jack Creek	Ben Lomond
Space Gp.	= R3m(160)	R3m(160)
a	= 15.9523(15)	15.9800(15) Å
c	= 7.1466(2)	7.1504(2) Å
V	= 1574.9(3)	1581.3(3) Å ³
Z	= 3	3
D _x	= 3.12	3.17 g/cm ³
ϵ	= 1.638(2)	1.642(2)
ω	= 1.660(2)	1.668(2)

X-ray Powder Diffraction Analysis

The X-ray powder diffraction data were collected using an automated Siemens D500 Kristallflex diffractometer, employing CuK α radiation ($\lambda = 1.54059$ Å), a diffracted beam graphite monochromator and a scintillation detector. The incident beam apertures (I, II and III) had 1° divergence and the monochromator and detector apertures were 0.05 and 0.15°, respectively. This combination of divergence and receiving slits yielded an instrumental profile breadth of 0.083° 2 θ for the 311 reflection of silicon powder (National Bureau of Standards, Standard Reference Material 640b).

Because of the small amount of sample available for analysis, the tourmaline powders were sprinkled on a Sie-

mens quartz zero background plate which had previously been coated with a thin layer of vaseline. The process of sprinkling and shaking off the excess was repeated until a uniform, thin coating was achieved. The external Si powder standard (SRM 640b) was prepared in the same way.

The data for each sample were collected in a series of three step scans over the range 10-100° 2 θ , using a 0.012° 2 θ step and counting time of 10s per step. The sample holder was rotated 90° for the third scan to evaluate the effects of preferred orientation. With the exception of the 220 reflection, which underwent only a modest increase in intensity no other reflections showed intensity changes related to sample orientation. Thus, the particle orientation appears to be well-randomized by this sample mounting technique.

The raw diffraction data were stripped of background and K α ₂ reflections, smoothed and searched for diffraction maxima using the Siemens software package. Each diffraction pattern was then manually edited to remove peaks due to impurities in the samples and add peaks missed by the peak marking routine. A microcomputer spread sheet was used to calibrate the peak positions using the Si external standard data, and to compute the means and standard deviations of the position and intensity of the reflections (Table 3).

The unit cell parameters were refined (Table 2) and the reflections indexed using 74 of the best resolved peaks, a CuK α ₁ wavelength of 1.54059 Å, and the least squares refinement program (Appleman & Evans, 1973) supplied as part of the Siemens software package. The parameters F₃₀ (Smith & Synder, 1979) and M₂₀ (DeWolff, 1968) are given in Table 3.

Table 3.
X-ray Powder Diffraction Data

Jack Creek					Ben Lomond				
2 θ _{exp}	2 θ _{calc}	I/I ₀	d _{exp}	$\Delta 2\theta$	2 θ _{exp}	I/I ₀	d _{exp}	hk l	
11.082(10)	11.084	2 (1)	7.98	-0.002	11.068	0.4	7.99	1 1 0	
13.922(10)	13.940	28 (5)	6.36	-0.018	13.922	23	6.36	1 0 1	
17.828 (5)	17.844	14 (2)	4.97	-0.016	17.822	11	4.97	0 2 1	
19.259 (6)	19.259	11 (2)	4.60	0.000	19.227	11	4.61	3 0 0	
21.043(13)	21.054	39 (8)	4.22	-0.011	21.029	36	4.22	2 1 1	
22.274(10)	22.273	85 (8)	3.99	0.001	22.239	62	3.99	2 2 0	
25.738 (1)	25.731	33 (2)	3.459	0.006	25.713	38	3.462	0 1 2	
26.371 (3)	26.372	7 (0)	3.377	-0.001	26.340	5	3.381	1 3 1	
28.093(12)	28.093	0.9 (3)	3.174	0.000	28.082	1	3.175	2 0 2	
28.679 (6)	28.684	3 (0)	3.110	-0.005	28.641	2	3.114	4 0 1	
29.615 (8)	29.608	9 (1)	3.014	0.007	29.563	7	3.019	4 1 0	
30.267 (7)	30.284	40 (3)	2.951	-0.017	30.255	40	2.952	1 2 2	
30.831 (0)	30.837	5 (1)	2.898	-0.006	30.793	6	2.901	3 2 1	
					33.627	0.2	2.663	3 3 0	
34.274(10)	34.287	3 (0)	2.614	-0.013	34.247	3	2.616	3 1 2	
34.800(10)	34.783	100 (0)	2.576	0.017	34.732	100	2.581	0 5 1	
36.149(10)	36.140	0.6 (2)	2.483	0.009	36.098	2	2.486	0 4 2	
36.617(12)	36.615	2 (0)	2.452	0.002	36.568	6	2.455	2 4 1	
37.706 (2)	37.732	5 (1)	2.384	-0.026	37.742	10	2.382	0 0 3	
37.903(11)	37.915	11 (0)	2.372	-0.012	37.862	12	2.374	2 3 2	

Table 3 (continued)

Jack Creek					Ben Lomond			
$2\theta_{\text{exp}}$	$2\theta_{\text{calc}}$	I/I ₀	d _{exp}	$\Delta 2\theta$	$2\theta_{\text{exp}}$	I/I ₀	d _{exp}	hkl
38.362 (4)	38.371	13 (0)	2.344	-0.009	38.309	12	2.348	5 1 1
39.095(12)	39.090	2 (0)	2.302	0.005	39.024	2	2.306	6 0 0
39.465(22)	39.446	0.4 (1)	2.281	0.019				1 1 3
40.765(19)	40.755	1 (0)	2.212	0.010	40.688	2	2.216	5 2 0
41.258(10)	41.270	6 (1)	2.186	-0.012	41.210	11	2.189	5 0 2
41.699 (8)	41.694	7 (0)	2.164	0.005	41.630	9	2.168	4 3 1
42.708(11)	42.699	4 (0)	2.115	0.009	42.675	7	2.117	3 0 3
42.870 (0)	42.865	3 (0)	2.108	0.005	42.821	3	2.111	4 2 2
44.415(13)	44.414	31 (2)	2.038	0.000	44.346	34	2.041	1 5 2
44.837(10)	44.814	7 (0)	2.020	0.023	44.753	7	2.023	1 6 1
45.446 (9)	45.449	2 (0)	1.9941	-0.003	45.361	3	1.9977	4 4 0
47.387(11)	47.390	16 (1)	1.9169	-0.003	47.314	21	1.9197	3 4 2
47.769 (3)	47.771	3 (0)	1.9025	-0.002	47.664	3	1.9064	7 0 1
48.666 (2)	48.677	3 (0)	1.8695	-0.011	48.613	6	1.8714	4 1 3
49.206 (7)	49.199	4 (0)	1.8502	0.007	49.116	6	1.8534	6 2 1
49.802 (7)	49.790	1 (0)	1.8294	0.012	49.699	1	1.833	7 1 0
50.217(30)	50.231	0.5 (3)	1.8153	-0.015	50.152	5	1.8175	6 1 2
51.433(18)	51.464	2 (0)	1.7752	-0.031	51.411	3	1.7759	3 3 3
51.537 (2)	51.536	2 (1)	1.7719	0.001	51.482	2	1.7736	1 0 4
52.557(20)	52.535	0.8 (3)	1.7399	0.022	52.414	0.3	1.7443	6 3 0
52.893 (1)	52.889	1 (0)	1.7296	0.004	52.864	3	1.7305	0 2 4
52.982(13)	52.959	1 (0)	1.7269	0.023				0 7 2
53.299(22)	53.310	0.5 (2)	1.7174	-0.011	53.191	0.8	1.7206	5 4 1
54.225(17)	54.218	1 (0)	1.6902	0.007	54.198	3	1.691	2 1 4
54.304(10)	54.287	2 (0)	1.6879	0.017				2 6 2
54.641(14)	54.632	0.3 (1)	1.6783	0.009	54.524	0.2	1.6817	0 8 1
55.437(20)	55.456	9 (0)	1.6561	-0.020	55.371	13	1.6579	6 0 3
55.955(15)	55.932	7 (0)	1.6420	0.023	55.832	11	1.6453	2 7 1
56.752(19)	56.744	0.3 (1)	1.6208	0.008	56.647	0.3	1.6236	5 2 3
					56.734	0.5	1.6213	1 3 4
57.764(10)	57.747	10 (1)	1.5948	0.017	57.629	15	1.5982	5 5 0
58.076(14)	58.079	4 (0)	1.5870	-0.003	58.014	5	1.5885	4 0 4
58.147 (0)	58.145	3 (0)	1.5852	0.002				4 5 2
58.475(11)	58.475	1 (0)	1.5771	0.000	58.369	1	1.5797	8 1 1
59.326 (5)	59.330	0.4 (1)	1.5565	-0.005	59.276	0.9	1.5577	3 2 4
59.719 (8)	59.721	2 (0)	1.5472	-0.002	59.612	3	1.5497	4 6 1
60.271 (6)	60.241	2 (0)	1.5343	0.030	60.122	3	1.5378	9 0 0
60.523(21)	60.500	2 (0)	1.5285	0.023				4 4 3
60.631 (9)	60.629	2 (0)	1.5261	0.002	60.533	3	1.5283	7 2 2
60.931 (4)	60.951	1 (1)	1.5193	-0.020	60.841	1	1.5213	7 3 1
61.462(30)	61.464	3 (1)	1.5074	-0.002	61.363	3	1.5096	8 2 0
61.824(15)	61.784	6 (3)	1.4994	0.040	61.707	8	1.502	0 5 4
62.988(15)	62.991	1 (0)	1.4745	-0.004	62.925	2	1.4758	2 4 4
63.049(10)	63.053	1 (0)	1.4732	-0.004				1 8 2
64.109(13)	64.121	6 (1)	1.4514	-0.012				7 1 3
64.200(18)	64.184	7 (0)	1.4496	0.016	64.092	12	1.4517	5 1 4
65.043(17)	65.055	2 (0)	1.4328	-0.012	64.921	3	1.4352	7 4 0
65.449(26)	65.427	0.7 (2)	1.4249	0.022	65.308	0.4	1.4276	3 7 2
65.609 (6)	65.613	2 (0)	1.4218	-0.005	65.601	7	1.422	0 1 5
65.734(14)	65.736	3 (1)	1.4194	-0.002				1 9 1

Table 3 (continued)

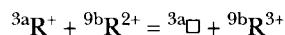
Jack Creek					Ben Lomond			
$2\theta_{\text{exp}}$	$2\theta_{\text{calc}}$	I/I _o	d _{exp}	$\Delta 2\theta$	$2\theta_{\text{exp}}$	I/I _o	d _{exp}	hkl
66.482(15)	66.474	5 (0)	1.4052	0.008	66.402	7	1.4067	6 3 3
66.555(21)	66.536	5 (1)	1.4039	0.019				4 3 4
					66.752	0.4	1.4002	2 0 5
67.961(29)	67.939	0.4 (3)	1.3782	0.022	67.891	0.9	1.3795	1 2 5
68.069(34)	68.060	0.7 (1)	1.3763	0.009				3 8 1
68.848 (2)	68.846	0.3 (1)	1.3626	0.002	68.744	1	1.3644	1 6 4
69.208(19)	69.207	4 (0)	1.3564	0.001	69.074	6	1.3587	10 0 1
70.058 (2)	70.048	1 (0)	1.3420	0.010	69.921	2	1.3443	9 1 2
70.389 (4)	70.346	0.4 (2)	1.3365	0.043				9 2 1
70.803(21)	70.824	3 (0)	1.3296	-0.021	70.680	3	1.3317	6 6 0
					70.953	3	1.3273	5 5 3
71.123(16)	71.122	3 (1)	1.3245	0.001	71.026	0.5	1.3261	7 0 4
71.348(34)	71.359	0.9 (4)	1.3209	-0.011	71.318	0.5	1.3214	0 4 5
71.988(19)	71.951	5 (0)	1.3107	0.037	71.804	6	1.3136	10 1 0
72.253(16)	72.247	2 (0)	1.3065	0.005				6 2 4
					72.166	2	1.3079	8 3 2
72.477(29)	72.484	1 (0)	1.3031	-0.007	72.426	0.9	1.3038	2 3 5
72.598 (8)	72.601	0.8 (1)	1.3012	-0.004				5 7 1
73.304(26)	73.307	0.5 (2)	1.2904	-0.003				9 0 3
73.440(19)	73.424	0.7 (1)	1.2883	0.016	73.267	1	1.2909	0 10 2
73.709 (4)	73.718	0.4 (0)	1.2843	-0.009	73.569	0.7	1.2864	8 4 1
74.200(33)	74.186	2 (0)	1.2770	0.014	74.037	3	1.2794	9 3 0
74.418(20)	74.420	3 (0)	1.2738	-0.002	74.288	1	1.2757	8 2 3
74.548(17)	74.536	2 (0)	1.2719	0.012				2 9 2
74.740(22)	74.712	3 (0)	1.2691	0.028	74.627	5	1.2708	5 0 5
75.592(11)	75.585	0.5 (2)	1.2568	0.007	75.474	0.8	1.2586	5 4 4
					75.734	3	1.2549	4 2 5
76.681 (7)	76.686	0.2 (0)	1.2417	-0.005	76.576	0.3	1.2432	0 8 4
76.769 (5)	76.743	0.4 (2)	1.2405	0.026				7 5 2
76.933(14)	76.917	0.8 (2)	1.2383	0.016				1 5 5
77.067(10)	77.032	2 (0)	1.2365	0.035	76.875	2	1.2391	0 11 1
77.716(10)	77.724	0.6 (1)	1.2278	-0.008	77.637	2	1.2288	7 4 3
77.786 (2)	77.781	0.7 (1)	1.2268	0.005				2 7 4
77.828 (0)	77.839	0.5 (0)	1.2263	-0.011				4 8 2
78.129(22)	78.126	0.4 (1)	1.2223	0.003	77.978	0.3	1.2243	2 10 1
78.590(10)	78.586	0.2 (1)	1.2163	0.004	78.435	0.4	1.2183	8 5 0
79.131(14)	79.102	0.3 (0)	1.2093	0.029	79.010	0.8	1.2109	3 4 5
79.205(28)	79.216	0.4 (2)	1.2084	-0.011	79.073	0.5	1.2101	7 6 1
79.965(14)	79.960	0.3 (3)	1.1988	0.005	79.869	0.5	1.2	8 1 4
80.590(20)	80.588	0.2 (2)	1.1911	0.002	80.515	0.4	1.192	0 0 6
81.040 (6)	81.044	0.2 (1)	1.1856	-0.004	80.913	0.3	1.1871	4 6 4
81.273 (8)	81.272	1 (0)	1.1828	0.001	81.195	3	1.1837	6 1 5
81.374(14)	81.385	1 (0)	1.1816	-0.011				11 1 1
81.663(20)	81.670	0.3 (2)	1.1781	-0.007	81.622	0.3	1.1786	1 1 6
82.122(16)	82.124	0.3 (2)	1.1727	-0.002	82.007	0.5	1.174	7 3 4
82.193 (9)	82.181	0.3 (0)	1.1719	0.011				10 2 2
83.166 (7)	83.145	0.3 (0)	1.1606	0.021				6 6 3
83.244(19)	83.258	0.2 (1)	1.1597	-0.014	83.061	0.2	1.1618	6 7 2
83.433(32)	83.428	0.4 (1)	1.1576	0.005	83.342	0.5	1.1586	0 7 5
83.556(21)	83.541	0.5 (1)	1.1562	0.015				10 3 1

Table 3 (continued)

Jack Creek					Ben Lomond			
$2\theta_{exp}$	$2\theta_{calc}$	I/I _o	d _{exp}	$\Delta 2\theta$	$2\theta_{exp}$	I/I _o	d _{exp}	hk l
84.008(14)	83.994	1 (0)	1.1511	0.014	83.838	2	1.153	12 0 0
84.187(17)	84.220	1 (0)	1.1491	-0.033	84.058	2	1.1505	10 1 3
84.495(35)	84.503	0.2 (1)	1.1457	-0.008				2 6 5
84.887(25)	84.890	0.2 (1)	1.1414	-0.003				2 2 6
85.054(26)	85.067	0.3 (1)	1.1396	-0.013	84.885	0.5	1.1414	11 2 0
85.413(17)	85.406	0.4 (2)	1.1357	0.007	85.238	0.7	1.1376	1 11 2
86.338(10)	86.365	0.4 (2)	1.1259	-0.027	86.222	1	1.1271	9 3 3
86.411 (2)	86.422	0.6 (2)	1.1251	-0.011				1 9 4
86.762(11)	86.759	0.2 (2)	1.1215	0.003	86.607	0.4	1.1231	6 8 1
87.533(25)	87.548	0.3 (2)	1.1136	-0.015	87.385	0.2	1.1151	3 10 2
87.722(17)	87.717	0.5 (2)	1.1117	0.005				4 5 5
87.807(11)	87.829	0.5 (2)	1.1108	-0.022	87.639	0.5	1.1125	9 5 1
88.122(19)	88.112	0.2 (1)	1.1077	0.010	88.030	0.2	1.1086	4 1 6
88.287 (4)	88.279	0.2 (1)	1.1060	0.008	88.088	0.2	1.108	10 4 0
88.571(24)	88.561	0.3 (1)	1.1032	0.010	88.411	0.1	1.1048	3 8 4
88.794(12)	88.787	0.2 (1)	1.1010	0.007				8 0 5
89.630(21)	89.630	0.4 (1)	1.0929	0.000	89.463	0.4	1.0945	10 0 4
89.946(22)	89.967	0.2 (1)	1.0899	-0.021	89.762	0.4	1.0916	1 12 1
					90.182	0.2	1.0876	
90.649(10)	90.642	0.4 (1)	1.0832	0.007				8 5 3
90.710 (5)	90.699	0.5 (0)	1.0827	0.011	90.536	0.8	1.0843	9 2 4
90.748(15)	90.755	0.5 (1)	1.0823	-0.007	90.575	1	1.0839	8 6 2
91.826 (6)	91.824	0.2 (0)	1.0724	0.002	91.631	0.3	1.0742	5 9 2
91.960 (5)	91.993	0.3 (0)	1.0712	-0.034	91.854		1.0722	1 8 5
92.094(23)	92.105	0.3 (1)	1.0700	-0.011				3 11 1
92.810(18)	92.838	1 (0)	1.0636	-0.028				5 7 4
93.060(38)	93.063	0.3 (0)	1.0614	-0.003				6 4 5
93.467 (8)	93.458	0.2 (1)	1.0578	0.009	93.375	0.6	1.0586	6 0 6
93.621(20)	93.626	0.2 (1)	1.0565	-0.005	93.726	0.2	1.0556	9 6 0
93.884(23)	93.908	0.2 (0)	1.0542	-0.024				8 4 4
93.963(29)	93.964	0.2 (1)	1.0536	-0.001				12 1 2
94.133(18)	94.134	0.1 (0)	1.0521	-0.001	93.970	0.2	1.0535	3 7 5
94.244(16)	94.246	0.1 (1)	1.0512	-0.002	94.440	0.1	1.0495	13 0 1
94.547(18)	94.529	0.2 (1)	1.0486	0.018				5 2 6
95.321(11)	95.319	0.2 (1)	1.0421	0.002	95.106	0.7	1.0439	12 2 1
					95.774	0.2	1.0384	12 0 3
96.090(11)	96.110	0.2 (0)	1.0358	-0.020				11 3 2
96.412(28)	96.393	0.3 (2)	1.0332	0.019	96.164	0.6	1.0352	5 10 1
97.074(18)	97.073	0.9 (1)	1.0279	0.001	96.902	2	1.0293	11 2 3
97.138(10)	97.130	0.9 (2)	1.0275	0.008	96.949	2	1.0289	0 11 4
97.742(24)	97.754	0.2 (1)	1.0227	-0.012				4 4 6
97.916(35)	97.924	0.4 (1)	1.0213	-0.008	97.685	1	1.0231	13 1 0
98.176(20)	98.208	0.4 (1)	1.0193	-0.032	98.034	0.5	1.0204	2 10 4
98.337 (4)	98.323	0.8 (1)	1.0181	0.014	98.253	2	1.0187	1 0 7
98.423(12)	98.436	0.8 (1)	1.0174	-0.014	98.277	2	1.0185	9 1 5
98.527(25)	98.549	0.9 (2)	1.0166	-0.022	98.343	1	1.018	11 4 1
99.356(17)	99.346	0.2 (0)	1.0103	0.010				2 12 2
99.394(13)	99.405	0.2 (0)	1.0100	-0.011				0 2 7
"F30 = 104 (0.009, 32)" M20 = 68					"F30 = 156 (0.006, 32)" M20 = 152			

Discussion

These schorls, as is the case with many tourmalines, are alkali cation-deficient and Al-rich (Foit & Rosenberg, 1977). Their compositions primarily reflect the presence of the alkali-defect substitution, a substitution, whereby an alkali-cation deficiency in the 9-coordinated $3a$ site is charge compensated by the substitution of trivalent for divalent cations in the larger octahedral $9b$ site according to the equation:



where $R^+ = Na$, $R^{2+} = Mg$ and Fe^{2+} , and $R^{3+} = Al$ and Fe^{3+} .

The tourmaline unit cell parameters have been shown (Rosenberg & Foit, 1979, Foit & Rosenberg, 1979 and Foit, 1989) to be a strong function of the occupancy of the octahedral sites, especially that of the larger $9b$ site. The unit cell parameters and cell volume (Table 2) of Ben Lomond schorl are larger than those of the Jack Creek schorl because the Ben Lomond schorl contains a higher percentage of Fe, the largest cation occupying these sites. Similarly, Andreasburg schorl (Fortier & Donnay, 1975), which contains even more octahedrally coordinated Fe than either the Jack Creek or Ben Lomond schorls, has still larger unit cell parameters ($a = 15.992$ and $c = 7.190 \text{ \AA}$).

The refractive indices of Ben Lomond schorl are slightly higher than those of Jack Creek due to its moderately higher Fe-content. However, the refractive indices and birefringence of both fall near the middle of the range reported for blue-green, green schorls (Heinrich, 1965).

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