Tables and figures

Table 1. End-member species for tourmaline group [99H1, 91N1] (group VIIIC08).

Silicate	(X)	(Y_3)	(Z_6)	T_6O_{18}	$(BO_3)_3$	V_3	W	Refs.
Alkali tourmalines								
Elbaite	Na	$Li_{1.5}Al_{1.5}$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	[a]
Dravite	Na	Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	[a]
Chromdravite	Na	Mg_3	Cr_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	83R1
Schörl	Na	$Fe^{2+}{}_3$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	[a]
Olenite[b]	Na	Al_3	Al_6	Si_6O_{18}	$(BO_3)_3$	O_3	(OH)	86S1
Buergerite	Na	$Fe^{3+}{}_3$	Al_6	Si_6O_{18}	$(BO_3)_3$	O_3	F	66D1
Povondraite[c]	Na	$Fe^{3+}{}_3$	$Fe^{3+}_4Mg_2$	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O	93G2
Calcic tourmalines								
Uvite	Ca	Mg_3	Al_5Mg	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F	29K1, 77D1
Hydroxy feruvite [b, d]	Ca	$Fe^{2+}{}_3$	Al_5Mg	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	89G2
Liddicoatite	Ca	Li_2Al	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F	77D2
X-site vacant tourmalines								
Rossmanite		$LiAl_2$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	98S1
Foitite[b]		$Fe^{2+}{}_2Al$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	93M1
Magnesiofoitite		Mg_2Al	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)	99H1
Verplanckite $Ba_4Mn_2Si_4O_{12}(OH,H_2O)_3Cl_3$								73K1, 91N1

[a] The definition of these end-members are lost in the mists of time;
[b] These end-members are modified from the originally suggested formulae to produce proper end-members;
[c] The original end-member **ferridravite** [79W1] was redefined as povondraite [93G2] because the initially assumed site populations were incorrect and did not correspond to the Fe^{3+}-equivalent of dravite. In [99H1] was suggested that Mg ordered at the Z-site should be part of the end-member formula;
[d] This species was originally defined as **feruvite**, but it has (OH) at O1 whereas uvite has F at O1, hence the name feruvite was modified to **hydroxy feruvite**.

Table 2. Atomic sites and thermal parameters.

a) Dravite[5], having space group R3m [93H1].

Atom	Site	*x*	*y*	*z*	$B_{eq} \cdot 10^4$ [Å^2]
X	3a	0	0	0.15920	211(8)
Y	9b	0.93867(3)	0.06133(3)	0.5643(4)	112(3)
Z	18c	0.73849(4)	0.70217(4)	0.5386(4)	71(2)
Si	18c	0.81018(3)	0.80835(3)	0.9280(4)	61(2)
B	9b	0.11000(9)	0.89000(9)	0.3819(5)	83(8)
O1	3a	0	0	0.6989(5)	124(7)
O2	9b	0.06109(7)	0.93891(7)	0.4156(4)	123(6)
O3	9b	0.86947(8)	0.13053(8)	0.4381(5)	140(6)
O4	9b	0.09300(8)	0.90601(8)	0.9989(5)	119(6)
O5	9b	0.90733(8)	0.09267(8)	0.0212(4)	114(6)
O6	18c	0.81568(9)	0.80578(9)	0.7059(4)	99(5)
O7	18c	0.71512(9)	0.71494(9)	0.0059(4)	99(5)
O8	18c	0.73016(9)	0.79077(9)	0.3674(4)	107(5)

Table 2 (cont.)

b) Verplanckite[34)], having hexagonal structure with space group P6/mmm [73K1].

Atom	Site	Coordination number	*x*	*y*	*z*	*B* [Å^2]
X(Mn,Ti,Fe)	6l	5	0.2606(4)	0.5212	0	1.0(2)
Si	12o	4	0.4440(4)	0.8880	0.274(2)	1.2(2)
O1	24r	4	0.160(1)	0.499(1)	0.197(3)	2.3(4)
O2	6i	4	1/2	0	0.206(5)	0.9(8)
O3	6m	4	0.441(2)	0.882	1/2	8(2)
Oh4(= OH,O)	2c	3	1/3	2/3	0	3(2)
Ba1	6j	8.4	0.3484(3)	0	0	2.9(1)
Ba2	6m	8.8	0.2164(2)	0.4328	1/2	2.2(1)
Cl1	2d	3	1/3	2/3	1/2	5(1)
0.3 · Cl2	12o	3	0.142(2)	0.284	0.118(6)	2(1)
0.6 · Cl3	6k	4	0.301(2)	0	1/2	5(1)

For footnotes [5)] and [34)] see Table 3.

Table 3. Crystal structures and lattice parameters[a)].

Silicate	*T* [K]	Space Group	Lattice parameters [Å]		Refs.
			a	*c*	
Elbaite[1)]	RT	R3m	15.837	7.101	97G1
Elbaite[2)]	RT	R3m	15.903	7.115	97G1
Al-rich elbaite[3)]	RT	R3m	15.802(31)	7.08609(92)	82G1
Mn-rich elbaite[4)]	RT	R3m	15.951(2)	7.116(2)	86S2
Dravite[5)]	RT	R3m	15.947(2)	7.214(1)	93H1
Chromdravite[6)]	RT	R3m	16.11	7.27	83R1
Ferridravite[7)]	RT	R3m	16.20(2)	7.47(1)	79W1
Schörl[8)]	RT	R3m	15.992(2)	7.190(1)	75F1
Olenite[9)]	RT	R3m	15.803(3)	7.086(1)	86S1
Olenite[10)]	RT	R3m	15.5996(8)	7.0224(6)	02M2
Olenite[11)]	RT	R3m	15.6329(8)	7.0365(6)	02M2
Buergerite[12)]	RT	R3m	15.869(2)	7.188(1)	69B1, 71T1
Buergerite[13)]	RT	R3m	15.967(2)	7.126(1)	93M1
Povondraite[14)]	RT	R3m	16.186(2)	7.444(1)	93G2
Uvite[15)]	RT	R3m	15.942(3)	7.205(2)	85T1
Hydroxy feruvite[16)]	RT	R3m	16.012(2)	7.245(2)	89G2
Liddicoatite[17)]	RT	R3m	15.867(4)	7.135(4)	77D2
Tourmaline[18)]	RT	R3m	15.935(1)	7.164(1)	99B1
Foitite[19)]	RT	R3m	15.967(2)	7.126(1)	93M1
Tourmaline[20)]	RT	R3m	15.896(15)	7.132(6)	87T1
Tourmaline[21)]	RT	R3m	15.869(11)	7.130(6)	87T1
Tourmaline[22)]	RT	R3m	15.805(38)	7.143(20)	87T1
Tourmaline[23)]	RT	R3m	15.828(9)	7.110(6)	87T1
Tourmaline[24)]	RT	R3m	15.942(3)	7.205(2)	87T1
Tourmaline[25)]	RT	R3m	15.822(2)	7.0949(4)	01H1
Tourmaline[26)]	RT	R3m	15.827(2)	7.1024(8)	01H1
Tourmaline[27)]	RT	R3m	15.939(1)	7.146(1)	99B1

Table 3 (cont.)

Silicate	*T* [K]	Space Group	Lattice parameters [Å]		Refs.
			a	*c*	
Tourmaline[28)]	RT	R3m	15.965(1)	7.199(1)	99B1
Tourmaline[29)] (synthetic olenite)	RT	R3m	15.626(10)	7.017(6)	00S1
Tourmaline[30)]	RT	R3m	15.951(1)	7.24(1)	62B1
Alkali-free tourmaline[31)]	RT	R3m	15.884(2)	7.128(1)	79R1
Alkali-free tourmaline[32)]	RT	R3m	15.847(5)	7.108(3)	79R1
X-site vacant Al tourmaline[33)]	RT	R3m	15.690(6)	7.039(5)	01W1
Verplanckite[34)]	RT	P6/mmm	16.398(10)	7.200(4)	73K1

a) The names of tourmalines were kept as in original papers (except Hydroxy feruvite);

1) $(Na_{0.86}K_{0.09}Ca_{0.05})(Li_{0.99}Mg_{0.27}Mn_{0.23}Fe^{2+}_{0.10}Al_{1.41})Al_{6.00}B_{2.93}Si_{6.00}O_{27.26}(OH)_{3.64}F_{0.10}$;

2) $(Na_{0.98}K_{0.02})(Li_{0.80}Mg_{0.28}Mn_{0.34}Fe^{2+}_{0.20}Fe^{3+}_{0.38}Al_{1.00})Al_{6.0}B_{3.00}(Si_{5.82}Al_{0.18})O_{27.54}(OH)_{3.32}$;

3) $(Na_{0.46}K_{0.01}Ca_{0.08}\square_{0.45})(Al_{2.18}Li_{0.53}Mn_{0.22}Fe^{3+}_{0.02}Ti_{0.005})(Al_{6.00}B_{2.96}Si_{6.09}O_{27}(O_{1.47}OH_{2.44}F_{0.09})$;

4) $(Na_{0.716}K_{0.006}Ca_{0.031})(Li_{0.686}Mn_{1.221}Fe_{0.004}Ti_{0.015}Al_{1.039})Al_6B_{2.94}Si_{5.661}Al_{0.339}OH_{3.929}F_{0.449}$; (no. of ions on the basis of (O,OH,F) = 31);

5) $^{X}(Na_{0.814}Ca_{0.009}K_{0.014}\square_{0.163})^{Y}(Mg_{1.301}Mn_{0.003}Fe^{2+}_{0.051}Fe^{3+}_{0.560}Cr_{0.006}Ti_{0.030}Al_{0.985})^{Z}(Al_{5.090}Mg_{0.910})(BO_3)_3Si_6O_{18}(O,OH)_4$;

6) $(Na_{0.97}Ca_{0.03})(Mg_{2.57}Mn_{0.03}V_{0.22}Al_{0.16}Ti_{0.02})(Cr_{4.71}Fe^{3+}_{1.08}Al_{0.21})(B_{2.91}Al_{0.09})(Si_{5.81}Al_{0.19})O_{27}(O_{0.23}OH_{3.77})$;

7) $(Na_{0.80}K_{0.24})(Mg_{1.58}Fe^{2+}_{1.15})(Fe^{3+}_{5.49}Al_{0.51})Si_6B_3(O,OH)_{30}(OH,F)$;

8) $Na_{2.63}Ca_{0.34}K_{0.03})(Fe^{2+}_{4.92}Al_{1.33}Fe^{2+}_{1.25}\square_{0.52}Mg_{0.32}Ca_{0.21}Ti^{4+}_{0.20}Li_{0.20}Mn^{2+}_{0.05})(Al_{16.82}Fe^{2+}_{1.18})B_{9.00}Si_{18.00}O_{81.89}(F,OH)_{11.11}$;

9) $(Na_{0.51}K_{0.01}Ca_{0.05}(Al_{2.91}Mn_{0.07}Fe_{0.02}Ti_{0.01})Al_6B_3Si_6O_{27}(O_{2.53}OH_{1.44}F_{0.03})$;

10) $Na_{0.8}Al_{2.9}Al_6[Si_{3.8}B_{2.2}O_{18}](B_3O_9)(OH,O)_4$;

11) $Na_{0.7}Al_{2.9}Al_6[Si_{4.2}B_{1.8}O_{18}](B_3O_9)(OH,O)_4$;

12) $(Na_{2.49}K_{0.05}Ca_{0.39}\square_{0.07})(Fe^{3+}_{6.93}Fe^{2+}_{0.56})Ti_{0.22}Mg_{0.10}Mn_{0.06}Al_{0.97}\square_{0.16})Al_{18.00}B_{9.00}(Si_{17.20}B_{0.80})(O_{88.63}OH_{1.39}F_{0.08})F_{3.00}$;

13) $(Na_{2.49}K_{0.05}Ca_{0.39}\square_{0.07})(Mg_{6.30}Al_{2.65}\square_{0.05})B_{9.00}(Al_{16.32}M_{1.57}\square_{0.11})(Si_{17.20}B_{0.80})(O_{88.53}OH_{1.39}F_{0.08})F_{3.00}$;

14) $(Na_{0.80}K_{0.26})(Fe^{3+}_{2.28}Fe^{2+}_{0.27}Mg_{0.53})(Fe^{3+}_{4.29}Mg_{1.36}Al_{0.32})B_3Si_{5.96}O_{27.88}(OH)_{3.12}$;

15) Composition [wt %]: SiO_2-37.09; B_2O_3-11.2; Al_2O_3-30.95; Fe_2O_3-0.72; MnO-1.27; CaO-3.68; MgO-12.87; Na_2O-1.08; Li_2O-0.36;

16) $(Ca_{0.62}Na_{0.39}K_{0.01})$ $(Fe^{2+}_{1.53}Mg_{1.21}Ti_{0.29}Mn_{0.01})(Al_{4.72}Mg_{0.82}Fe^{3+}_{0.34}Fe^{2+}_{0.12})(BO_3)_3(Si_{5.83}Al_{0.10})O_{18}(OH)_4$;

17) $(Ca_{0.72}Na_{0.27})(Li_{1.59}Al_{1.13}Fe_{0.11}Ti_{0.05}Mn_{0.04}Mg_{0.03}\square_{0.05})Al_{6.00}B_{3.00}Si_{6.02}(O_{27.27}(OH)_{2.73})(F_{0.87}(OH)_{0.13})$;

18) $Ca_{0.017}Na_{0.533}K_{0.040}Li_{0.001}Fe^{2+}_{0.685}Fe^{3+}_{0.361}Mn_{0.003}Cr_{0.002}V_{0.014}Ti_{0.083}B_{3.03}Si_{6.035}Al_{6.573}O_{31}F_{0.106}Cl_{0.001}H_{3.041}$;

19) $^{X}(\square_{0.75}Na_{0.25})^{Y}(Li_{0.22}Mg_{0.05}Fe^{2+}_{1.60}Mn^{2+}_{0.24}Al_{0.89})^{Z}Al_6Si_{6.01}O_{18}(BO_3)_3(OH)_4$;

20) Composition [wt %]: SiO_2-35.90; B_2O_3-10.0; Al_2O_3-35.85; Fe_2O_3-6.00; MnO-1.18; MgO-0.09; Na_2O-4.75; Li_2O-2.58; CaO-0.02;

21) Composition [wt %]: SiO_2-36.34; B_2O_3-11.5; Al_2O_3-44.23; Fe_2O_3-1.48; MnO-1.33; MgO-0.15; Na_2O-2.41; Li_2O-1.51; CaO < 0.02;

22) Composition [wt %]: SiO_2-37.09; B_2O_3-11.8; Al_2O_3-44.47; Fe_2O_3-0.71; MnO-1.22; MgO-0.01; Na_2O-2.04; Li_2O-2.01; CaO < 0.02;

23) Composition [wt %]: SiO_2-35.93; B_2O_3-11.0; Al_2O_3-45.45; Fe_2O_3-2.30; MnO-1.49; MgO-0.10; Na_2O-2.22; Li_2O-1.88; CaO < 0.02;

24) Composition [wt %]: SiO_2-37.09; B_2O_3-11.2; Al_2O_3-30.95; Fe_2O_3-0.72; MnO-1.27; MgO-12.87; Na_2O-1.08; Li_2O-0.36; CaO-3.68;

25) $(Na_{0.516}Ca_{0.092}K_{0.009})(Al_{0.542}Li_{0.458})_3(Al_{0.989}Li_{0.011})_6(Si_{0.928}Al_{0.036}B_{0.037})_6B_3O_{27}[(OH)_{2.895}F_{0.499}O_{0.606}]$;

26) $(Na_{0.517}Ca_{0.105})(Al_{0.576}Li_{0.424})_3(Al_{0.958}Li_{0.042})_6(Si_{0.938}Al_{0.003}B_{0.059})_6B_3O_{27}[(OH)_{2.921}F_{0.484}O_{0.595}]$;

27) $(Na_{0.471}K_{0.029}Ca_{0.368})Al_{5.245}Li_{0.018}Ti_{0.034}Fe^{2+}_{0.293}Fe^{3+}_{0.864}Mg_{2.207}Mn_{0.012}Cr_{0.003}V_{0.001}B_{3.048}Si_{6.164}F_{0.495}Cl_{0.004}H_{3.028}O_{31}$;

28) $Na_{0.711}K_{0.043}Ca_{0.100}Al_{7.014}Li_{0.006}Ti_{0.049}Fe^{2+}_{1.005}Fe^{3+}_{0.179}Mg_{0.844}Mn_{0.003}Cr_{0.003}V_{0.007}B_{3.011}Si_{5.657}F_{0.302}Cl_{0.001}H_{3.466}O_{31}$;

[29] $(Na_{0.65}\square_{0.35})(Al_{2.72}\square_{0.28})(Al_{5.42}Si_{0.58})[Si_{3.73}B_{2.27}O_{18}](BO_3)_3(OH)_{3.87}O_{0.13}$;
[30] $Na_{0.39}K_{0.01}Ca_{0.60}B_{3.00}Mg_{3.55}Fe_{0.03}Al_{5.58}Si_{5.58}O_{30.61}F_{0.49}H_{3.00}$;
[31] $\square_{0.92}Mg_{0.08}(Mg_{1.98}Al_{1.02})Al_6(Si_{5.59}Al_{0.41})(BO_3)_3O_{17.74}(OH)_{4.28}$, synthesized at 600 °C;
[32] $\square_{0.04}Mg_{0.96}(Mg_{1.52}Al_{1.48})Al_6(Si_{5.23}Al_{0.77})(BO_3)_3O_{19.60}(OH)_{2.40}$, synthesized at 450 °C;
[33] $(\square_{0.96}Na_{0.04})Al_3(Al_{5.83}\square_{0.29})[(Si_{4.49}B_{1.51})O_{18}](BO_3)_3(OH)_{3.21}O_{0.79}$;
[34] $(Mn_{4.06}Ti_{1.50}Fe_{0.29})Ba_{11.27}Si_{12}O_{36}O_{2.20}Cl_{8.84}(H_2O)_{7.05}$;
[35] $(Na_{2.49}Ca_{0.39}K_{0.05}\square_{0.07})(Fe^{3+}{}_{5.99}Al_{2.65}Ti_{0.18}Mg_{0.08}Mn_{0.05}\square_{0.05})B_{9.00}(Al_{16.32}Fe^{3+}{}_{0.93}Fe^{2+}{}_{0.56}\square_{0.11})$ $(Ti_{0.04}Mg_{0.02}Mn^{2+}{}_{0.02})(Si_{17.20}B_{0.80})O_{88.53}F_{3.08}(OH)_{1.39}$;
[36] $(Ca_{1.56}Na_{1.35}Sr_{0.05}K_{0.04})(Mg_{7.78}Fe^{2+}{}_{1.22})B_{9.00}(Al_{14.91}Fe^{2+}{}_{1.20}Fe^{3+}{}_{1.19}\square_{0.33}Ti_{0.28}Ca_{0.08}Mn^{2+}{}_{0.01})(Si_{17.94}B_{0.06})O_{81.39}$ $(OH)_{9.21}F_{1.56}$;
[37] $(Na_{1.40}Ca_{1.30}\square_{0.24}K_{0.06})(Mg_{6.65}Fe^{2+}{}_{2.01}Fe^{3+}{}_{0.34})B_{9.00}(Al_{13.39}Fe^{3+}{}_{3.77}Ti_{0.06}\square_{0.24})(Si_{17.76}B_{0.24})O_{81.29}(OH)_{12.17}F_{0.29}$;
[38] $Na_{0.518}K_{0.004}Ca_{0.099}Li_{1.562}Fe^{3+}{}_{0.001}Mn_{0.015}Al_{7.894}B_{3.280}Si_{5.690}Ti_{0.001}O_{31}H_{2.895}F_{0.499}$;
[39] $Na_{0.532}K_{0.004}Ca_{0.104}Li_{1.550}Fe^{3+}{}_{0.001}Mn_{0.022}Al_{7.807}B_{3.202}Si_{5.797}O_{31}H_{2.977}F_{0.464}$;
[40] $Na_{0.528}K_{0.004}Ca_{0.128}Li_{1.773}Fe^{3+}{}_{0.007}Mn_{0.023}Al_{7.617}B_{3.367}Si_{5.753}H_{2.921}F_{0.484}O_{31}$;
[41] $Na_{0.523}K_{0.002}Ca_{0.078}Li_{1.557}Mn_{0.030}Mg_{0.005}Zn_{0.001}Al_{7.794}B_{3.052}Cr_{0.001}B_{3.052}Ti_{0.009}H_{3.325}F_{0.651}O_{31}$;
[42] $Na_{0.374}K_{0.006}Ca_{0.511}Fe^{3+}{}_{0.008}Cr_{0.001}Mg_{3.309}Al_{5.744}B_{3.039}Ti_{0.004}Si_{5.961}O_{31}H_{3.127}F_{0.615}$;
[43] $^{X}(Na_{0.40}Ca_{0.29}\square_{0.31})^{Y}(Al_{2.42}Li_{0.36}\square_{0.22})^{Z}(Al_{5.92}\square_{0.08}B_3)^{T}(Si_{4.86}B_{1.06}Al_{0.08})O_{27}[F_{0.06}(OH)_{3.31}O_{0.63}]$;
[44] Natural sample of Uncle Sam Gulch (Montana);
[45] Natural sample from Arizona having 18.1 mol % FeO;
[46] Composition [wt %]: Na_2O-1.84; CaO-0.05; MgO-4.39; FeO-4.50; MnO-0.20; TiO_2-0.23; Al_2O_3-38.80; SiO_2-37.23 (B content not mentioned, probably $B_{3.0}$ per f.u.);
[47] Composition [wt %]: Na_2O-2.45; CaO-0.43; K_2O-0.03; FeO-0.91; MnO-3.17; ZnO-0.04; Li_2O-1.54; Al_2O_3-39.50; SiO_2-37.10; F-1.50 (B content not mentioned, probably $B_{3.0}$ per f.u.);
[48] $Na_{0.522}K_{0.002}Ca_{0.007}Al_{6.915}Ti_{0.010}Fe^{2+}{}_{1.774}Mg_{0.386}Mn_{0.033}Li_{0.121}B_{3.006}Si_{5.895}F_{0.181}H_{3.390}$;
[49] $Na_{0.671}K_{0.006}Ca_{0.036}Al_{6.483}Ti_{0.127}Fe^{2+}{}_{1.385}Fe^{3+}{}_{0.073}Mg_{1.007}Mn_{0.014}Cr_{0.001}Zn_{0.006}Li_{0.010}B_{3.005}Si_{5.938}F_{0.299}H_{3.166}$;
[50] $Na_{0.697}Ca_{0.153}Al_{5.858}Ti_{0.037}Fe^{2+}{}_{1.497}Fe^{3+}{}_{0.264}Mg_{1.474}Mn_{0.006}Cr_{0.001}Li_{0.001}B_{3.028}Si_{6.025}F_{0.013}H_{3.326}$;
[51] $(Na_{0.797}K_{0.013}Ca_{0.062})Al_{6.437}Ti_{0.075}Fe^{3+}{}_{2.624}Mg_{0.042}Mn_{0.016}Cr_{0.001}Li_{0.016}B_{3.015}Si_{5.821}F_{0.836}Cl_{0.003}H_{0.285}$;
[51a] For samples 48-51 the composition is for 31 O atoms;
[52] $(Na_{0.66}Ca_{0.10}K_{0.01})(Ti_{0.10}Al_{0.62}Fe_{1.63}Mn_{0.02}Zn_{0.01}Mg_{0.84})Al_{6.00}(BO_3)_3Si_{6.00}O_{18}F_{0.25}OH_{3.50}$;
[53] $(Na_{0.82}Ca_{0.06}Fe^{2+}{}_{0.06}Mg^{2+}{}_{2.49}Ti^{4+}{}_{0.13}Al^{3+}{}_{0.28})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[54] $(Na_{0.62}Ca_{0.17}Fe^{2+}{}_{1.22}Mg^{2+}{}_{1.22}Ti^{4+}{}_{0.07}Al^{3+}{}_{0.35})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[55] $(Na_{1.00}Ca_{0.02}Fe^{2+}{}_{0.76}Al^{3+}{}_{1.20})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[56] $(Na_{0.90}Ca_{0.02}Mn^{2+}{}_{0.90}Fe^{2+}{}_{0.02}Al^{3+}{}_{0.92})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[57] $(Na_{0.75}Ca_{0.10}Mn^{2+}{}_{0.76}Fe^{2+}{}_{0.12}Al^{3+}{}_{0.92})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[58] $(Na^{+}{}_{0.55}Al^{3+}{}_{2.10})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[59] $(Na_{0.58}Ca_{0.05}Mn^{2+}{}_{0.09}Al^{3+}{}_{1.86})Al^{3+}{}_{6.0}Si_{6.0}$ (only cation content);
[60] $(Na_{0.35}Ca_{0.52})Mn^{2+}{}_{0.03}Fe^{2+}{}_{0.11}Al^{3+}{}_{1.29})Al_{6.0}Si_{6.0}$ (only cation content);
[61] $Na_{0.80}Mg_{1.14}Fe_{0.84}Al_{1.01}Al_{6.00}(Si_{5.61}Al_{0.39})(BO_3)_3$; see [67a];
[62] $Na_{0.03}Fe_{2.05}Al_{0.89}Ti_{0.06}Al_{6.00}(Si_{5.85}Al_{0.15})(BO_3)_3$; see [67a];
[63] $Na_{0.03}Cu_{0.03}Mn_{0.48}Al_{2.48}Al_{6.00}Si_{5.22}Al_{0.78}(BO_3)_3$; see [67a];
[64] $Na_{0.78}Mn_{0.64}Fe_{0.02}Al_{2.15}Al_{6.00}Si_{6.18}(BO_3)_3$; see [67a];
[65] $Na_{0.16}Fe_{1.62}Al_{1.38}Al_{6.00}Si_{6.00}(BO_3)_3$; see [67a];
[66] $Na_{0.73}Fe_{1.40}Al_{1.60}Al_{6.00}(Si_{5.18}Al_{0.82})(BO_3)_3$; see [67a];
[67] $Na_{0.48}Cu_{0.03}Fe_{0.61}Al_{2.37}Al_6(Si_{5.44}Al_{0.56})(BO_3)_3$; see [67a];
[67a] In samples [61-67] was assumed $(BO_3)^{3-}{}_3$ and the compositions were determined per 54 net negative charges;
[68] $(Na_{0.56}K_{0.01}Ca_{0.01})(Al_{0.59}Ti_{0.02}Cr_{<0.01}Fe_{2.27}Mn_{0.03}Ni_{<0.01}Zn_{0.02}Mg_{0.01})Al_{6.00}Si_{6.00}$ (only cation content);
[69] $Na_{0.77}Ca_{0.07}K_{0.01}[Li_{0.91}]Al_{7.53}Fe_{0.12}Mn_{0.43}Si_{6.00}$ (only cation content);
[70] $Na_{0.84}Ca_{0.03}Mg_{0.02}[Li_{0.62}]Al_{7.36}Fe_{0.63}Mn_{0.38}Si_{6.00}$. (only cation content);
[71] $(Na_{0.01}Ca_{0.40}Mg_{0.50})(Mg_{5.01}Fe^{2+}{}_{0.29}Al_{0.49}Fe^{3+}{}_{0.21})(B_{2.61}Al_{3.39})(Si_{5.38}Al_{0.62})[O_{25.98}(OH)_{3.99}F_{0.03}]$;
[72] Composition [wt %]: SiO_2 – 37.45; B_2O_3 – 11.51; Al_2O_3 – 41.41; Fe_t – 0.03; MnO – 0.05; TiO_2 – 0.01; ZnO – 0.15; CaO – 0.07; Na_2O – 1.88; K_2O – 0.01; F – 0.91;
[73] Composition [wt %]: SiO_2 – 37.72; B_2O_3 – 11.21; Al_2O_3 – 42.75; Fe_t – 0.01; MnO – 0.01; ZnO – 0.01; Cr_2O_3 – 0.01; CaO – 0.01; Na_2O – 1.85; K_2O – 0.01; Li_2O – 1.23; F – 0.46; OH – 0.14;

Table 4. Elastic constants of some tourmalines.

	Method	$c_{ij} \cdot 10^{11}$ [N/m^2]						Refs.
		c_{11}	c_{33}	c_{44}	c_{66}	c_{13}	c_{14}	
Uvite[15)]	Pulse echo	3.016	1.698	0.655	1.028	0.47	–0.089	85T1
Tourmaline[20)]	Elastic wave velocity	3.052	1.764	0.646	0.984	0.51	–0.06	87T1
Tourmaline[21)]	Elastic wave velocity	2.958	1.733	0.636	0.963	0.45	–0.10	87T1
Tourmaline[22)]	Elastic wave velocity	3.000	1.738	0.652	0.969	0.42	–0.07	87T1
Tourmaline[23)]	Elastic wave velocity	3.011	1.746	0.654	0.973	0.43	–0.07	87T1
Tourmaline[24)]	Elastic wave velocity	3.016	1.698	0.655	1.028	0.47	–0.09	87T1
Tourmaline (natural)	Resonance method	2.72	1.65	0.65	1.16	0.35	–0.068	50M1
Tourmaline (natural)	Wedge method	3.04	1.76	0.65	1.08	0.35	–0.04	50B2
Tourmaline (natural)	Wedge method	2.63	1.51	0.595	1.01	0.49	–0.09	50B2
Tourmaline (natural)	Phase comparison method	3.050	1.764	0.648	0.984	0.51	–0.06	79O1

For samples tourmalines[20)-24)] (see Table 3 for composition), the estimated errors for c_{11}, c_{33}, c_{44}, c_{66} are 0.4 %, for c_{13} 4 % and for c_{14} 10 %. For uvite[15)] the estimated errors are 0.2 % for c_{11}, c_{33}; 0.3 % for c_{44}, c_{66}; 3 % for c_{11} and 6 % for c_{14}.

Table 5. Elastic modulus and Debye temperature.

Silicate	$\cdot 10^{11}$ N/m^2		Poisson ratio	Debye temperature Θ_D [K]	Refs.
	Bulk modulus K_H	Shear modulus G_H			
Uvite[15)]	1.226	0.826	0.224		85T1
Tourmaline[20)]	1.260	0.817	0.235	765.4	87T1
Tourmaline[21)]	1.213	0.798	0.229	766.1	87T1
Tourmaline[22)]	1.211	0.816	0.224	762.1	87T1
Tourmaline[23)]	1.217	0.819	0.225	763.0	87T1
Tourmaline[24)]	1.226	0.826	0.224	764.3	87T1

For footnotes (composition) [15)], [20-24)] see Table 3.

Table 6. Data obtained by ^{11}B and ^{29}Si MAS NMR spectroscopy.

Silicate	BO_3				BO_4				Refs.
	δ [ppm]	e^2Qq/h [MHz]	η	A [%]	δ [ppm]	e^2Qq/h [MHz]	η	A [%]	
^{11}B[a)]									
Tourmaline[38)]	19.4	2.9	0.14	97	0.0	0.1	0.8	3	99T1
Tourmaline[39)]	19.6	2.9	0.16	97	0.1	0.2	0.8	3	99T1
Tourmaline[40)]	19.9	2.9	0.14	97	0.0	0.1	0.7	3	99T1
Tourmaline[41)]	20	2.9	0.15	94	0.0	0.1	0.7	6	99T1
Tourmaline[42)]	20.1	2.9	0.16	100					99T1
Olenite[43)]	18.3	1.41	0.11		–0.6	0.3	$\cong 0$		02M1
Olenite[29)]	12.564			– [f)]	–0.613				00S1
	2.50								
Dravite (natural)	11.96			100					00S1
	0.82								

Table 6 (cont.)

Silicate	BO_3				BO_4				Refs.
	δ [ppm]	e^2Qq/h [MHz]	η	A [%]	δ [ppm]	e^2Qq/h [MHz]	η	A [%]	
^{29}Si[b)]									
Olenite (synthetic)	–88.7								02M2
Olenite[43)]	–90[c)]				–85[d)]				02M1

a) Chemical shift to ^{11}B reference of $NaBH_4$;
b) Relative to tetramethylsilane;
c) Silicon connected to two other Si atoms in hexagonal ring;
d) Silicon connected to one Si and one B atom;
e) $Na_{0.8}Al_{2.9}Al_6[Si_{3.8}B_{2.2}O_{18}]B_3O_9(OH,O)_4$. A small signal at –107.3 ppm typical for quartz was shown;
f) The ratio $BO_3/BO_4 = 0.96$; not all trigonal boron contributed to the BO_3 signal;
For footnote numbers of first column (sample composition) see Table 3.

Table 7. Hyperfine parameters obtained from ^{57}Fe NGR studies (selected data) of RT.

Silicate	Site	δ [mm/s]	ΔQ [mm/s]	DH [mm/s]	A [%]	Refs.
Tourmaline[44)]	Fe^{2+}(Y1)	1.087(2)	2.487(8)	0.140(6)	21.4	98F1
	Fe^{2+}(Y2)	1.087(2)	1.99(2)	0.20(4)	14.9	
	Fe^{2+}(Z)	1.035(8)	1.40(5)	0.32(2)	21.1	
	$Fe^{3+} – Fe^{2+}$(ED)	0.52(1)	0.83(3)	0.200	8.8	
	Fe^{3+}(Y)	0.385(3)	0.793(5)	0.200	33.9	
Tourmaline (synthetic, 500°C, 40 days, log $f_{O_2} = –31.6$)	Fe^{2+}(Y)	1.225(3)	2.886(6)	0.220(4)	58.8	98F1
	Fe^{2+}(Y)	1.276(8)	2.15(3)	0.220(4)	14.6	
	Fe^{3+}(Y)	0.408(7)	0.94(1)	0.22(1)	26.6	
Tourmaline (synthetic, 600°C, 20 days, log $f_{O_2} = –27.0$)	Fe^{2+}(Y)	1.108(7)	2.68(3)	0.15(3)	18.2	98F1
	Fe^{2+}(Y)	1.108(7)	2.2(1)	0.28(2)	45.7	
	Fe^{2+}(Z)	1.07(3)	1.800	0.160	5.6	
	Fe^{2+}(Y or Z)	0.40(1)	1.130	0.200	18.1	
	Fe^{3+}(Y)	0.34(1)	0.730	0.160	12.4	
Tourmaline (synthetic, 700°C, 8 days, log $f_{O_2} = –23.7$)	Fe^{2+}(Y)	1.120(4)	2.62(2)	0.16(1)	20.9	98F1
	Fe^{2+}(Y)	1.11(1)	2.09(1)	0.228(9)	60.5	
	Fe^{2+}(Z)	1.05(1)	1.75	0.160	7.5	
	Fe^{3+}(Y)	0.46(6)	0.8(1)	0.200	11.1	
Tourmaline (synthetic, 400°C, 140 days, log $f_{O_2} = –28.8$)	Fe^{2+}(Y)	1.225(2)	2.762(4)	0.40(1)	64.5	98F1
	Fe^{3+}(Y)	0.484(4)	0.908(8)	0.45(1)	35.6	
Tourmaline[45)]	Fe^{2+}(Y)	1.09	2.39	0.30	32	79S1
	Fe^{2+}(Z)	1.05	1.74	0.51	27	
	Fe^{3+}(Z)	0.46	0.82	0.42	32	
	$Fe^{2+}–Fe^{3+}$	0.86	1.21	0.42	9	

Table 7 (cont.)

Silicate	Site	δ [mm/s]	ΔQ [mm/s]	DH [mm/s]	A [%]	Refs.
Fe-Mg-Al bearing	Fe^{2+}(Y)	1.093	2.412	0.33	38	93F1
Tourmaline[46)]	Fe^{2+}(Z)	1.051	1.823	0.43	30	
	Fe^{2+}–Fe^{3+}(ED)	0.682	1.204	0.44	16	
Elbaite[47)]	Fe^{2+}(Y)	1.048	2.469	0.32	45	93F1
	Fe^{2+}(Z)	1.131	2.332	0.32	55	
Schörl[48)]	Fe^{2+}(Y1)	1.10	2.49	0.24	39	98D1
	Fe^{2+}(Y2)	1.10	2.21	0.31	36	
	Fe^{2+}(Y3)	1.06	1.56	0.55	25	
Schörl[49)]	Fe^{3+}(Y or Si)	0.18	0.51	0.24	5	98D1
	Fe^{2+}(Y1)	1.08	2.49	0.24	43	
	Fe^{2+}(Y2)	1.09	2.21	0.28	23	
	Fe^{2+}(Y3)	1.06	1.66	0.51	29	
Schörl[50)]	Fe^{3+}(oct)	0.41	0.73	0.60	12	98D1
	Fe^{3+}-Fe^{2+}(ED)	0.79	1.08	0.50	6	
	Fe^{2+}(Y1)	1.09	2.53	0.24	36	
	Fe^{2+}(Y2)	1.09	2.33	0.26	27	
	Fe^{2+}(Y3)	1.05	1.83	0.47	19	
Buergerite[51)]	Fe^{3+}(oct)	0.37	1.24	0.33	70	98D1
	Fe^{3+}(oct)	0.35	0.90	0.31	30	

For footnotes of column 1 (sample composition) see Table 3.

Table 8. Assignment of the hydroxyl stretching bands (in cm^{-1}) in the IR spectrum of different tourmalines [88G2].

Silicate	OH1		OH3		
			AlAlLi	$AlAlM^{2+}$	AlAlAl
Dravite[53)]	MgMgMg	3738		3568	
Schörl[54)]	MgMgMg	3738			
	FeFeFe	3633		3553	
Elbaite[58, 59)]	AlAlLi	3650	3583	–	3464
Ca-Elbaite[60)]	AlAlLi	3680, 3650	3604, 3586	–	3507, 3473
Mn-Elbaite[56, 57)]	AlMnLi	3670	3594	3568	3492
Fe-Elbaite[55)]	AlFeLi	3692	3594	3558	3492

For footnotes (sample composition) see Table 3.

Table 9. Energies at room temperature, polarization and origin of bands [93T1].

Sample	Band	ν [cm^{-1}]	Polarization	Origin	
				Center	Transition
Fe^{2+}, Fe^{3+}- and Fe^{2+}, Ti^{4+}-bearing synthetic tourmalines					
Tourmaline[61)]	a	14000	σ	Fe^{2+}(Z) –Fe^{3+}(Y,Z), ECP[1)]	$^5T_{2g} \rightarrow {}^5E_g$
	b	9000	σ		
	c	≅14000	π	Fe^{2+}(Y,Z)	$^5T_{2g} \rightarrow {}^5E_g$
	d	≅9000	π		
	e	≅19000	σ	Fe^{2+}(Y) – Fe^{3+}(Y)	$Fe^{2+}Fe^{3+}$-CT[2)]
Tourmaline[65)]	f	13300	σ	Fe^{2+}(Y) – Fe^{3+}(Y,Z), ECP	$^5T_{2g} \rightarrow {}^5E_g$
	g	9300	σ		
Tourmaline[66)]	h	12500	σ	Fe^{2+}(Y) – Fe^{3+}(Z)	$Fe^{2+}Fe^{3+}$-CT
Tourmaline[62)]	i	22500	σ	Fe^{2+}(Y) – Ti^{4+}(Y)	$Fe^{2+}Ti^{4+}$-CT
	j	≅20000	σ	Fe^{2+}(Y) – Ti^{4+}(Z)	$Fe^{2+}Ti^{4+}$-CT
Fe^{3+} bearing synthetic tourmalines[3)]					
Tourmaline[67)]	a	20800 (21050)	σ	Fe^{3+}(Y)	$^6A_{1g} \rightarrow {}^4A_{1g}, {}^4E_g$
	b	18200 (18200)	σ = π	Fe^{3+}(Y)	$^6A_{1g} \rightarrow {}^4T_{2g}$
Mn^{3+} in Mn-bearing synthetic tourmalines					
Tourmaline[63)]	a	23500	σ		
	b	22000	π		$^5E_g \rightarrow {}^5T_{2g}$
	c	18000	σ > π		
	d	9800	σ		
Tourmaline[64)]	e	23250	σ		
	f	22000	π		$^5E_g \rightarrow {}^5T_{2g}$
	g	18700	σ		
	h	10860	σ		

[1)] ECP – exchange coupled pair; [2)] CT – charge transfer transitions; [3)] The ν values are at 297 K and 77 K (in parenthesis).- For footnotes [61) - 65)] (sample composition) see Table 3.

Table 10. Refractive indices.

Silicate	$n(\omega)$	$n(\varepsilon)$		Refs.
Mn-rich elbaite[4)]	1.649(1)	1.621(1)		86S2
Dravite[71)]	1.6375	1.626	uniaxial negative	66W1
Chromdravite[6)]	1.778	1.772	uniaxial negative	83R1
Ferridravite[7)]	1.800(3)	1.743(3)	uniaxial negative	79W1
Olenite[9)]	1.654(2)	1.635(2)		86S1
Povondraite[14)]	1.820(5)	1.751(3)	uniaxial negative	93G2
Hydroxy feruvite[16)]	1.687(1)	1.669(1)	uniaxial negative	89G2
Foitite[19)]	1.664(1)	1.642(1)	uniaxial negative	93M1
Liddicoatite[17)]	1.637	1.621	uniaxial negative	77D2
Alkali-free tourmaline[31)] (synthesized 600°C)	1.624(1)	1.605(1)	uniaxial negative	79R1
Alkali-free tourmaline[32)] (synthesized 450°C)	1.624(1)	1.607(1)	uniaxial negative	79R1