Table S1. Atom coordinates of the three tourmaline crystals of this study.

sample	atom	mul.		site occupancy			*x*/*a*	*y*/*b*	*z*/*c*	U_{eq}
1	*T*	1	Si	1			0.189816(18)	0.191865(17)	0.03998(4)	0.00494(7)
2	*T*	1	Si	1			0.19004(3)	0.19201(3)	0.04069(7)	0.00465(15)
12	*T*	1	Si	1			0.19000(2)	0.19197(2)	0.04066(7)	0.00493(11)
1	*B*	2	B	1			0.89095(5)	0.10905(5)	0.5869(2)	0.0055(2)
2	*B*	2	B	1			0.89081(11)	0.10919(11)	0.5864(4)	0.0069(5)
12	*B*	2	B	1			0.89063(7)	0.10937(7)	0.5862(4)	0.0057(4)
1	*X*	6	Na	0.23(8)	Ca	0.31(5)	0.0000	0.0000	0.8077(2)	0.0240(11)
2	*X*	6	Na	0.33(13)	Ca	0.44(8)	0.0000	0.0000	0.8056(3)	0.0249(12)
12	*X*	6	Na	0.51(11)	Ca	0.31(7)	0.0000	0.0000	0.8059(3)	0.0216(11)
1	*Y*	2	Al	0.649(4)	Li	0.351(4)	0.06125(2)	0.93875(2)	0.40487(10)	0.0070(2)
2	*Y*	2	Al	0.898(7)	Li	0.102(7)	0.06172(3)	0.93828(3)	0.41157(13)	0.0096(3)
12	*Y*	2	Al	0.826(6)	Li	0.174(6)	0.06177(3)	0.93823(3)	0.41110(13)	0.0084(3)
1	*Z*	1	Al	0.996(3)	Li	0.004(3)	0.26004(2)	0.29666(2)	0.43134(5)	0.00531(9)
2	*Z*	1	Al	0.983(5)	Li	0.017(5)	0.26054(4)	0.29736(4)	0.42919(8)	0.00475(18)
12	*Z*	1	Al	0.985(4)	Li	0.015(4)	0.26053(3)	0.29732(3)	0.42928(8)	0.00536(13)
1	O1	6	F	0.916(9)			0.0000	0.0000	0.2630(3)	0.0291(7)
2	O1	6	F	1.005(16)			0.0000	0.0000	0.2562(6)	0.0537(19)
12	O1	6	F	1.031(16)			0.0000	0.0000	0.2569(6)	0.0574(17)
1	O2	2	O	1			0.93980(4)	0.06020(4)	0.55116(18)	0.0133(2)
2	O2	2	O	1			0.93938(8)	0.06062(8)	0.5584(3)	0.0174(5)
12	O2	2	O	1			0.93952(6)	0.06048(6)	0.5581(3)	0.0173(4)
1	O3	2	O	1			0.13164(5)	0.86836(5)	0.53345(17)	0.0121(2)
2	O3	2	O	1			0.13424(8)	0.86576(8)	0.5313(3)	0.0112(4)
12	O3	2	O	1			0.13415(6)	0.86585(6)	0.5313(3)	0.0112(3)
1	H3	2	H	0.97(5)			0.1304(9)	0.8696(9)	0.646(4)	0.014
2	H3	2	H	1.06(8)			0.1311(13)	0.8689(13)	0.631(6)	0.013
12	H3	2	H	1.03(8)			0.1319(13)	0.8681(13)	0.633(5)	0.013
1	O4	2	O	1			0.90612(4)	0.09388(4)	0.96659(17)	0.00918(19)
2	O4	2	O	1			0.90704(8)	0.09296(8)	0.9684(3)	0.0085(4)
12	O4	2	O	1			0.90701(6)	0.09299(6)	0.9682(3)	0.0087(3)
1	O5	2	O	1			0.09362(4)	0.90638(4)	0.94384(16)	0.00964(19)
2	O5	2	O	1			0.09295(7)	0.90705(7)	0.9462(3)	0.0085(4)
12	O5	2	O	1			0.09302(6)	0.90698(6)	0.9467(3)	0.0089(3)
1	O6	1	O	1			0.18420(5)	0.19487(5)	0.26618(12)	0.00736(13)
2	O6	1	O	1			0.18648(9)	0.19658(9)	0.2655(2)	0.0075(3)
12	O6	1	O	1			0.18649(7)	0.19654(7)	0.26525(19)	0.0081(2)
1	O7	1	O	1			0.28626(5)	0.28665(5)	0.96249(10)	0.00644(13)
2	O7	1	O	1			0.28584(9)	0.28589(9)	0.96005(17)	0.0066(3)
12	O7	1	O	1			0.28574(7)	0.28577(7)	0.96036(16)	0.0067(2)
1	O8	1	O	1			0.26992(5)	0.20939(5)	0.60191(11)	0.00722(13)
2	O8	1	O	1			0.27036(10)	0.20966(10)	0.59935(17)	0.0076(3)
12	O8	1	O	1			0.27039(7)	0.20976(7)	0.59956(17)	0.0079(2)

Table S2a. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for tor1_1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
T	4(1)	5(1)	6(1)	0(1)	0(1)	2(1)
B	6(1)	6(1)	6(1)	0(1)	0(1)	3(1)
X	27(1)	27(1)	19(1)	0	0	13(1)
Y	5(1)	5(1)	10(1)	-1(1)	1(1)	1(1)
Z	6(1)	5(1)	5(1)	0(1)	-1(1)	3(1)
O(1)	36(1)	36(1)	15(1)	0	0	18(1)
O(2)	17(1)	17(1)	14(1)	0(1)	0(1)	15(1)
O(3)	11(1)	11(1)	4(1)	-1(1)	1(1)	-2(1)
O(4)	7(1)	7(1)	9(1)	1(1)	-1(1)	0(1)
O(5)	7(1)	7(1)	9(1)	1(1)	-1(1)	0(1)
O(6)	8(1)	7(1)	6(1)	0(1)	0(1)	3(1)
O(7)	5(1)	6(1)	7(1)	0(1)	1(1)	2(1)
O(8)	9(1)	5(1)	8(1)	-1(1)	-3(1)	4(1)

Table S2b. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for tor2_1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
T	4(1)	5(1)	5(1)	0(1)	0(1)	2(1)
B	8(1)	8(1)	6(1)	1(1)	-1(1)	4(1)
X	26(1)	26(1)	23(2)	0	0	13(1)
Y	7(1)	7(1)	12(1)	-1(1)	1(1)	2(1)
Z	6(1)	5(1)	4(1)	0(1)	-1(1)	3(1)
O(1)	74(3)	74(3)	14(2)	0	0	37(1)
O(2)	26(1)	26(1)	14(1)	0(1)	0(1)	23(1)
O(3)	11(1)	11(1)	3(1)	0(1)	0(1)	-1(1)
O(4)	7(1)	7(1)	8(1)	1(1)	-1(1)	0(1)
O(5)	6(1)	6(1)	9(1)	0(1)	0(1)	-1(1)
O(6)	7(1)	8(1)	5(1)	0(1)	1(1)	2(1)
O(7)	5(1)	6(1)	6(1)	0(1)	1(1)	1(1)
O(8)	10(1)	5(1)	9(1)	-1(1)	-2(1)	5(1)

Table S2c. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for tor12_1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
T	4(1)	4(1)	6(1)	0(1)	0(1)	2(1)
B	6(1)	6(1)	6(1)	0(1)	0(1)	3(1)
X	23(1)	23(1)	18(1)	0	0	12(1)
Y	6(1)	6(1)	12(1)	-1(1)	1(1)	2(1)
Z	7(1)	5(1)	5(1)	0(1)	0(1)	3(1)
O(1)	79(2)	79(2)	15(2)	0	0	39(1)
O(2)	26(1)	26(1)	14(1)	0(1)	0(1)	24(1)
O(3)	10(1)	10(1)	5(1)	0(1)	0(1)	-2(1)
O(4)	7(1)	7(1)	9(1)	1(1)	-1(1)	0(1)
O(5)	7(1)	7(1)	8(1)	1(1)	-1(1)	0(1)
O(6)	8(1)	7(1)	7(1)	-1(1)	1(1)	2(1)
O(7)	5(1)	6(1)	7(1)	0(1)	1(1)	2(1)
O(8)	10(1)	6(1)	8(1)	-1(1)	-3(1)	5(1)