Supporting Information

$Li_5Rb_2B_7O_{14}$: A New Congruently Melting Compound with Two Kinds of B–O One–dimensional Chains and Short UV Absorption Edge

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Figure S1. Powder XRD pattern of $Li_5Rb_2B_7O_{14}$.

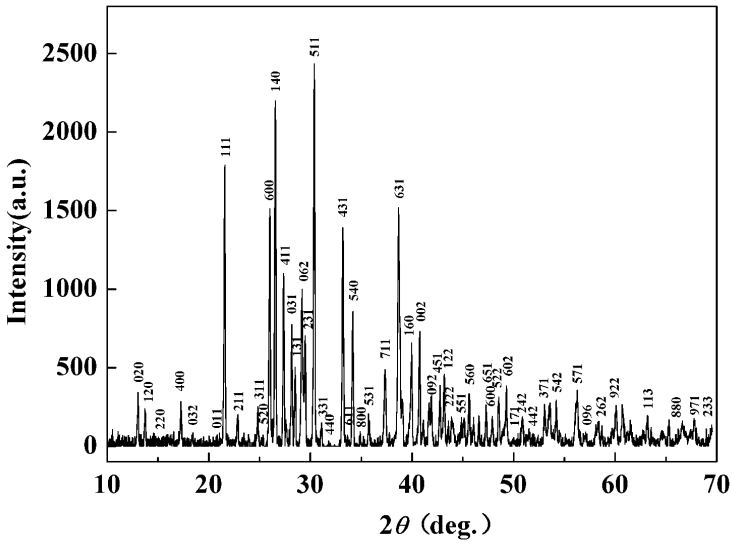

Figure S2. Experimental and calculated XRD patterns of the $Li_5Rb_2B_7O_{14}$.

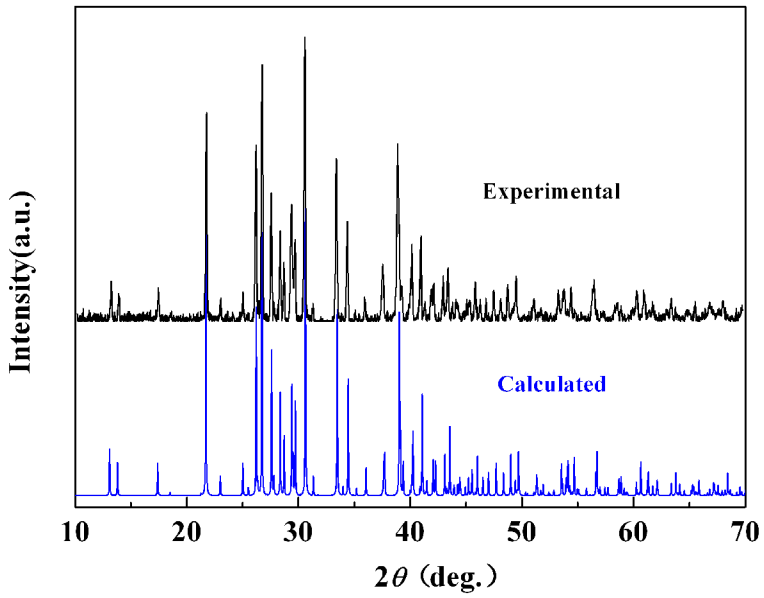

Figure S3. Powder XRD pattern of the $Li_5Rb_2B_7O_{14}$ samples before and after melting, respectively.

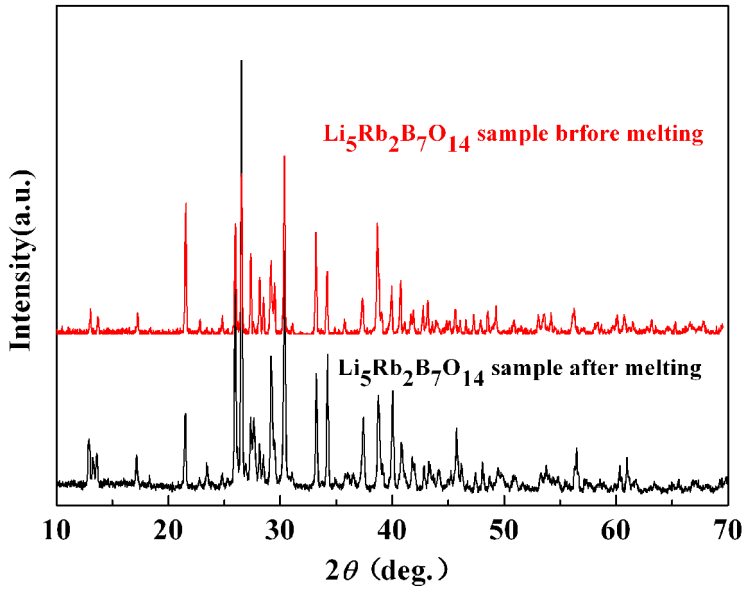

Figure S4. A representation of B–O structural building unit down *c* axis.

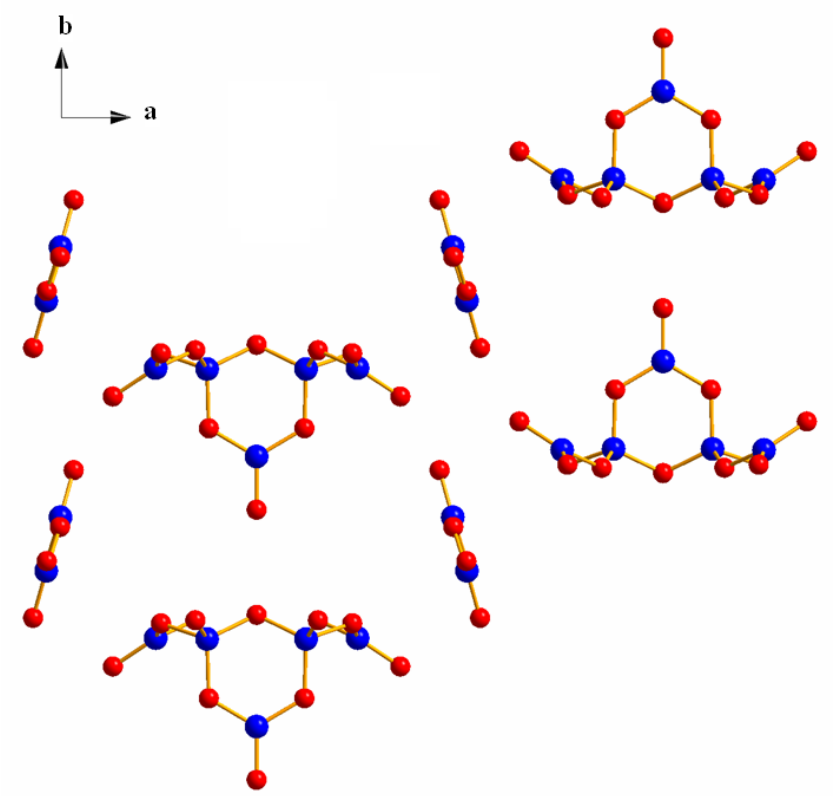

Figure S5. View of the structure of $Li_5Rb_2B_7O_{14}$ and cations coordination environments down *c* axis (orange, Li; green, Rb; blue, B; red, O; purple, BO_4 group; light blue, BO_3 group).

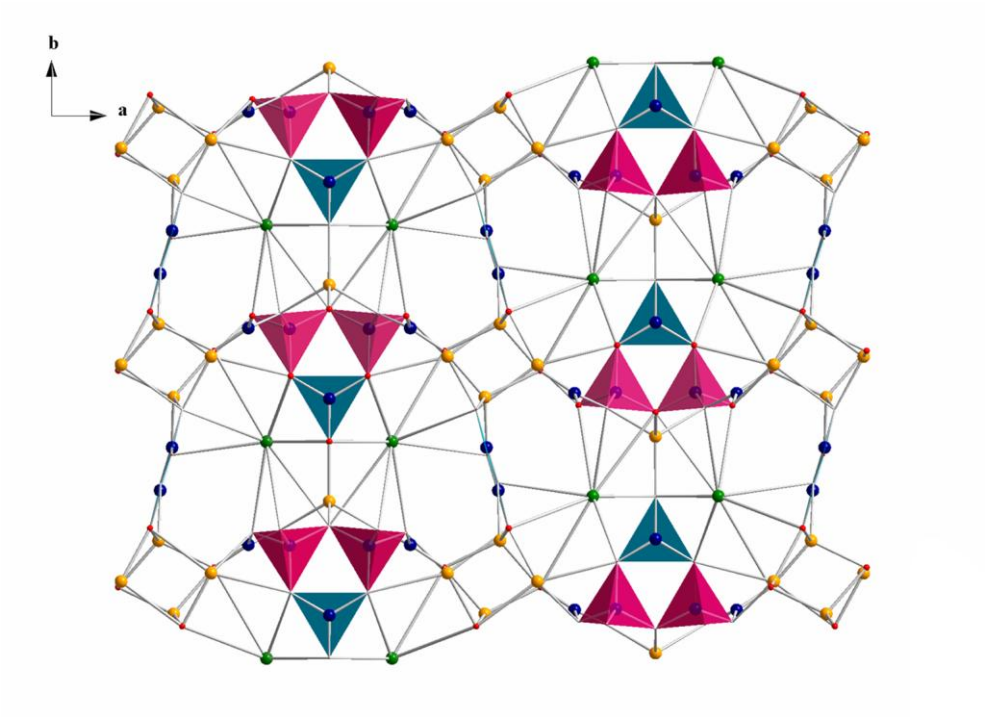

Figure S6. $Rb(1)O_{10}$ groups are interconnected via sharing edges infinite 1D double chains along *c* axis (green, Rb; red, O).

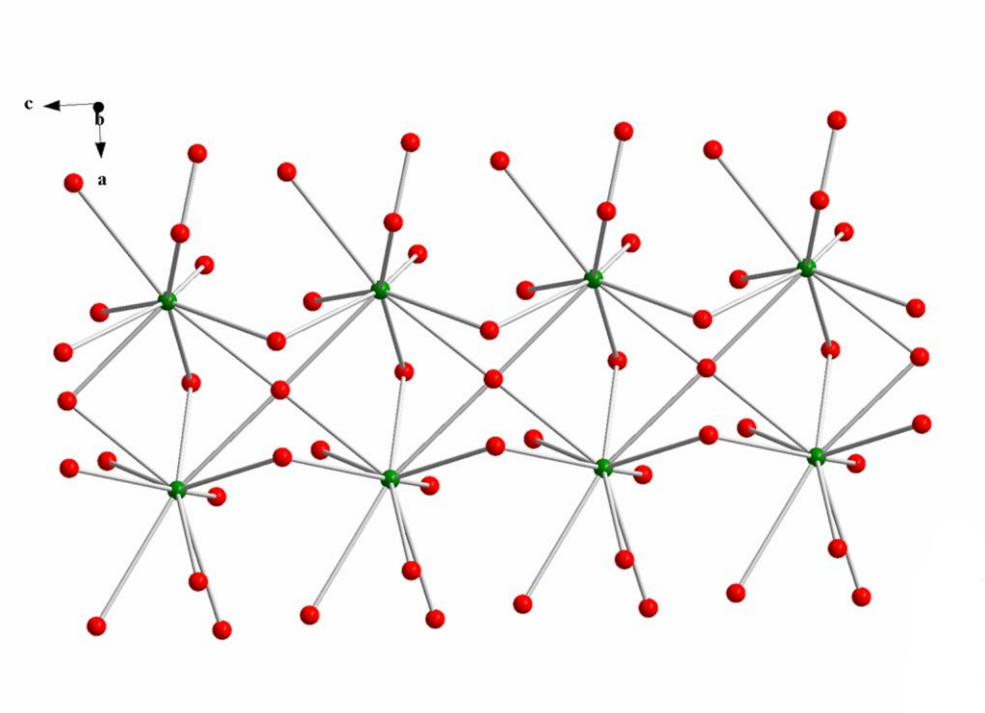

Figure S7. Infrared spectroscopy of the $Li_5Rb_2B_7O_{14}$ sample.

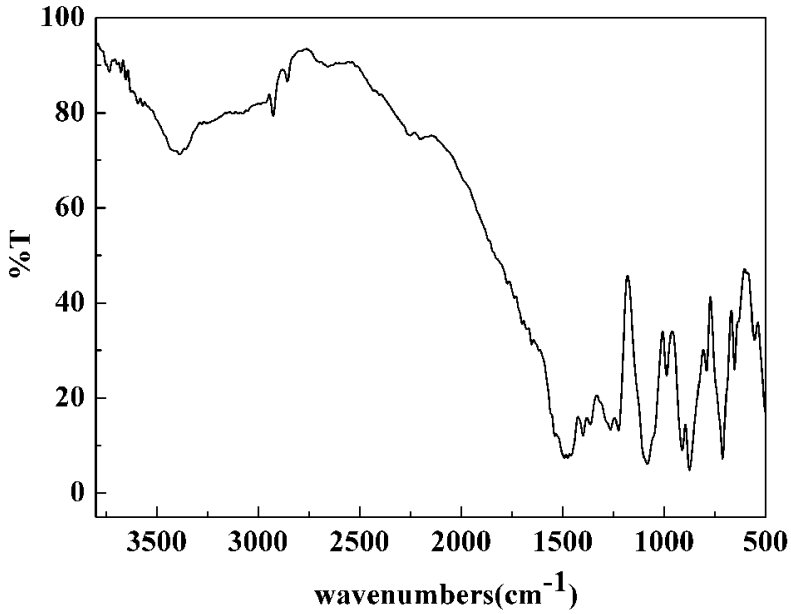

Figure S8. UV-VIS-NIR diffuse-reflectance spectrum of $Li_5Rb_2B_7O_{14}$.

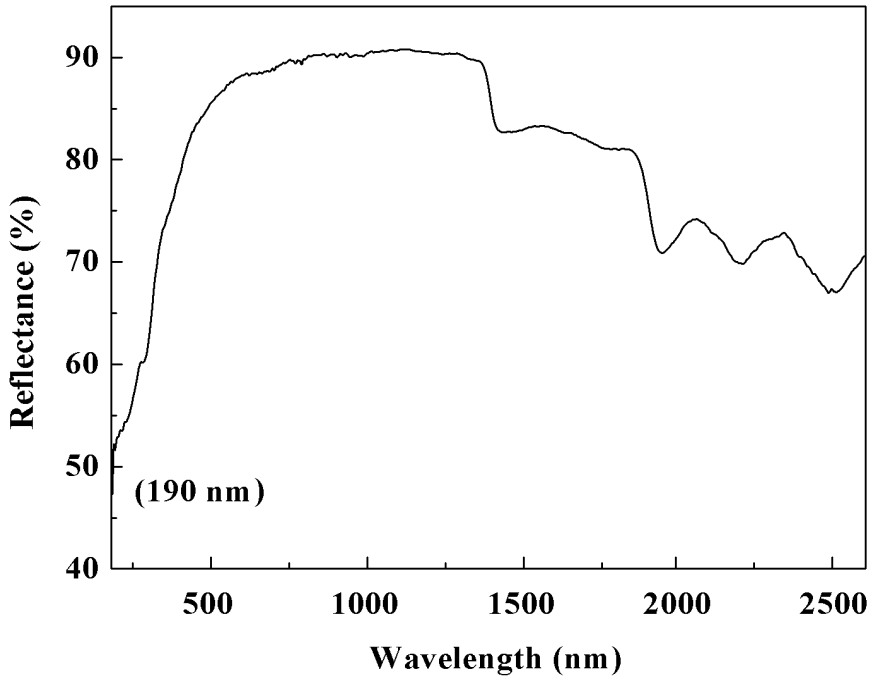

Figure S9. Phase matching curve, i.e., particle size vs SHG intensity, data for $Li_5Rb_2B_7O_{14}$. The curve is drawn to guide the eye and is not a fit to the data.

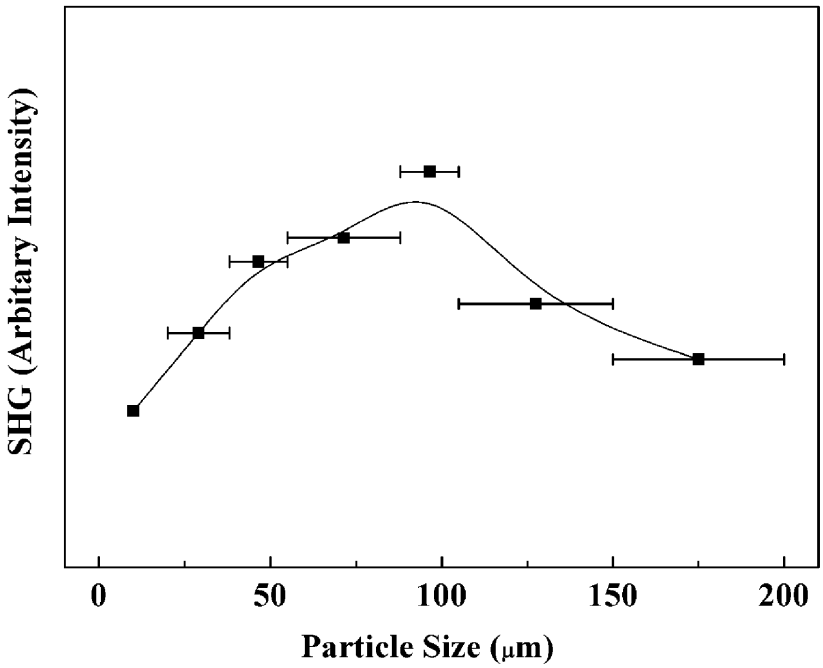

Table S1. Selected bond distances (Å) and angles (deg) for $Li_5Rb_2B_7O_{14}$.

Rb(1)-O(1)#1	2.919(6)	B(4)-O(5)	1.377(6)
Rb(1)-O(1)	2.967(6)	B(4)-O(7)	1.345(5)
Rb(1)-O(6)#2	2.978(3)	B(4)-O(6)#1	1.394(7)
Rb(1)-O(2)#1	3.093(3)	Li(1)-O(1)	1.874(8)
Rb(1)-O(3)	3.097(3)	Li(1)-O(5)#11	1.935(8)
Rb(1)-O(2)	3.099(3)	Li(1)-O(5)#12	1.935(8)
Rb(1)-O(5)#2	3.123(3)	Li(1)-O(4)#2	1.967(18)
Rb(1)-O(4)#2	3.299(3)	Li(2)-O(2)	2.574(8)
Rb(1)-O(7)	3.300(2)	Li(2)-O(7)	1.930(10)
Rb(1)#9-O(8)	3.336(3)	Li(2)-O(6)	1.958(8)
B(1)-O(1)	1.333(6)	Li(2)-O(8)#7	1.912(7)
B(1)-O(2)	1.390(4)	Li(2)-O(8)#8	2.387(8)
B(1)-O(2)#6	1.390(4)	Li(2)-O(7)#5	2.479(10)
B(2)-O(2)	1.483(4)	Li(3)-O(8)	1.915(11)
B(2)-O(4)	1.447(4)	Li(3)-O(3)#7	1.941(7)
B(2)-O(5)	1.479(7)	Li(3)-O(7)#7	1.942(6)
B(2)-O(6)	1.481(6)	Li(3)-O(7)#12	1.947(6)
B(3)-O(3)	1.402(6)	Li(3)-O(8)#5	2.574(11)
B(3)-O(8)	1.294(5)	O(1)-Li(1)-O(5)#4	117.3(5)
B(3)-O(3)#3	1.415(9)	O(1)-Li(1)-O(5)#5	117.3(5)
O(1)#1-Rb(1)-O(1)	96.471(12)	O(5)#4-Li(1)-O(5)#5	105.1(6)
O(1)#1-Rb(1)-O(6)#2	107.55(8)	O(1)-Li(1)-O(4)#2	112.9(8)
O(1)-Rb(1)-O(6)#2	84.07(8)	O(5)#4-Li(1)-O(4)#2	100.9(5)
O(1)#1-Rb(1)-O(2)#1	46.20(8)	O(5)#5-Li(1)-O(4)#2	100.9(5)

O(1)-Rb(1)-O(2)#1	111.54(10)	O(8)#9-Li(2)-O(7)	106.2(4)
O(6)#2-Rb(1)-O(2)#1	148.99(8)	O(8)#9-Li(2)-O(6)	143.3(5)
O(1)#1-Rb(1)-O(3)	146.06(12)	O(7)-Li(2)-O(6)	106.5(4)
O(1)-Rb(1)-O(3)	116.45(12)	O(8)#9-Li(2)-O(8)#10	96.5(3)
O(6)#2-Rb(1)-O(3)	70.24(7)	O(7)-Li(2)-O(8)#10	97.1(4)
O(2)#1-Rb(1)-O(3)	120.25(7)	O(6)-Li(2)-O(8)#10	95.7(3)
O(1)#1-Rb(1)-O(2)	111.03(10)	O(8)#9-Li(2)-O(7)#7	84.7(3)
O(1)-Rb(1)-O(2)	45.82(8)	O(7)-Li(2)-O(7)#7	169.1(4)
O(6)#2-Rb(1)-O(2)	118.20(8)	O(6)-Li(2)-O(7)#7	63.2(3)
O(2)#1-Rb(1)-O(2)	90.30(6)	O(8)#10-Li(2)-O(7)#7	81.3(3)
O(3)-Rb(1)-O(2)	98.50(7)	O(8)#9-Li(2)-O(2)	104.4(3)
O(1)#1-Rb(1)-O(5)#2	65.06(8)	O(7)-Li(2)-O(2)	87.2(3)
O(1)-Rb(1)-O(5)#2	104.49(9)	O(6)-Li(2)-O(2)	61.1(2)
O(6)#2-Rb(1)-O(5)#2	45.67(6)	O(8)#10-Li(2)-O(2)	156.6(3)
O(2)#1-Rb(1)-O(5)#2	103.44(8)	O(7)#7-Li(2)-O(2)	90.2(3)
O(3)-Rb(1)-O(5)#2	97.02(7)	O(8)-Li(3)-O(3)#9	100.3(3)
O(2)-Rb(1)-O(5)#2	150.30(7)	O(8)-Li(3)-O(7)#9	101.6(4)
O(1)-Rb(1)-O(2)	45.82(8)	O(3)#9-Li(3)-O(7)#9	132.2(5)
O(6)#2-Rb(1)-O(2)	118.20(8)	O(8)-Li(3)-O(7)#5	110.3(4)
O(2)#1-Rb(1)-O(2)	90.30(6)	O(3)#9-Li(3)-O(7)#5	108.0(3)
O(3)-Rb(1)-O(2)	98.50(7)	O(7)#9-Li(3)-O(7)#5	103.2(3)
O(1)#1-Rb(1)-O(5)#2	65.06(8)	O(8)-Li(3)-O(8)#7	155.6(3)
O(1)-Rb(1)-O(5)#2	104.49(9)	O(3)#9-Li(3)-O(8)#7	60.2(3)
O(6)#2-Rb(1)-O(5)#2	45.67(6)	O(7)#9-Li(3)-O(8)#7	84.5(3)
O(2)#1-Rb(1)-O(5)#2	103.44(8)	O(7)#5-Li(3)-O(8)#7	90.8(4)

O(3)-Rb(1)-O(5)#2	97.02(7)	O(1)-B(1)-O(2)#8	120.5(2)
O(2)-Rb(1)-O(5)#2	150.30(7)	O(1)-B(1)-O(2)	120.5(2)
O(1)#1-Rb(1)-O(4)#2	72.18(9)	O(2)#8-B(1)-O(2)	119.0(4)
O(1)-Rb(1)-O(4)#2	61.17(9)	O(4)-B(2)-O(5)	108.6(3)
O(6)#2-Rb(1)-O(4)#2	45.38(6)	O(4)-B(2)-O(6)	112.8(4)
O(2)#1-Rb(1)-O(4)#2	117.80(7)	O(5)-B(2)-O(6)	106.4(3)
O(3)-Rb(1)-O(4)#2	115.49(6)	O(4)-B(2)-O(2)	112.7(3)
O(2)-Rb(1)-O(4)#2	106.98(7)	O(5)-B(2)-O(2)	110.3(5)
O(5)#2-Rb(1)-O(4)#2	43.32(7)	O(6)-B(2)-O(2)	105.9(3)
O(1)#1-Rb(1)-O(7)	114.07(8)	O(8)-B(3)-O(3)	126.1(7)
O(1)-Rb(1)-O(7)	104.45(8)	O(8)-B(3)-O(3)#3	118.7(5)
O(6)#2-Rb(1)-O(7)	135.95(7)	O(3)-B(3)-O(3)#3	115.2(3)
O(2)#1-Rb(1)-O(7)	68.01(6)	O(7)-B(4)-O(5)	124.6(5)
O(3)-Rb(1)-O(7)	67.33(7)	O(7)-B(4)-O(6)#1	119.6(4)
O(2)-Rb(1)-O(7)	58.73(6)	O(5)-B(4)-O(6)#1	115.7(3)
O(5)#2-Rb(1)-O(7)	150.93(7)		
O(4)#2-Rb(1)-O(7)	165.44(7)		

Note. Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1	#2 x,y-1/2,z+1/2	#3 -x+1,-y+1/2,z+1/2
#4 -x+1/2,y-1/2,z-1/2	#5 x,y-1/2,z-1/2	#6 -x+1/2,y,z-1
#7 x,y,z-1	#8 -x+1/2,y,z	#9 -x+1,-y+1/2,z-1/2
#10 x,y+1/2,z-1/2	#11 -x+1,-y+1,z	#12 -x+1,-y,z
#13 x,y+1/2,z+1/2	#14 -x+1/2,y+1/2,z-1/2	

Table S2. Bond valence analysis of the $Li_5Rb_2B_7O_{14}$.[a,b]

Atoms	l	s	Atoms	l	s
Rb(1)-O(1)#1	2.919(6)	0.170	Li(1)-O(1)	1.874(8)	0.332
Rb(1)-O(1)	2.967(6)	0.149	Li(1)-O(5)#11	1.935(8)	0.282
Rb(1)-O(6)#2	2.978(3)	0.145	Li(1)-O(5)#12	1.935(8)	0.282
Rb(1)-O(2)#1	3.093(3)	0.106	Li(1)-O(4)#2	1.967(18)	0.258
Rb(1)-O(3)	3.097(3)	0.105	∑s		1.154
Rb(1)-O(2)	3.099(3)	0.104	Li(2)-O(2)	2.574(8)	0.05
Rb(1)-O(5)#2	3.123(3)	0.098	Li(2)-O(7)	1.930(10)	0.285
Rb(1)-O(4)#2	3.299(3)	0.061	Li(2)-O(6)	1.958(8)	0.265
Rb(1)-O(7)	3.300(2)	0.061	Li(2)-O(8)#7	1.912(7)	0.300
Rb(1)-O(8)	3.336(3)	0.055	Li(2)-O(8)#8	2.387(8)	0.083
∑s		1.054	Li(2)-O(7)#5	2.479(10)	0.065
B(1)-O(1)	1.333(6)	1.108	∑s		1.048
B(1)-O(2)	1.390(4)	0.950	Li(3)-O(8)	1.915(11)	0.297
B(1)-O(2)#6	1.390(4)	0.950	Li(3)-O(3)#7	1.941(7)	0.277
∑s		3.008	Li(3)-O(7)#7	1.942(6)	0.276
B(2)-O(2)	1.483(4)	0.739	Li(3)-O(7)#12	1.947(6)	0.273
B(2)-O(4)	1.447(4)	0.814	Li(3)-O(8)#5	2.574(11)	0.05
B(2)-O(5)	1.479(7)	0.747	∑s		1.173
B(2)-O(6)	1.481(6)	0.743	B(4)-O(5)	1.377(6)	0.984
∑s		3.043	B(4)-O(7)	1.345(5)	1.073
B(3)-O(3)	1.402(6)	0.92	B(4)-O(6)#1	1.394(7)	0.94
B(3)-O(8)	1.294(5)	1.231	∑s		2.997
B(3)-O(3)#3	1.415(9)	0.888			

∑s		3.039			

[a] Bond valences calculated with the program Bond Valence Calculator Version 2.00, Hormillosa, C., Healy, S., Stephen, T. McMaster University (1993).

[b] Valence sums calculated with the formula: $S_i = \exp[(R_0-R_i)/B]$, where S_i = valence of bond "i" and $B = 0.37$. Superscripts indicate the number of equivalent bonds for anions.