Supporting Information

A new lithium rubidium borate $Li_6Rb_5B_{11}O_{22}$ with isolated $B_{11}O_{22}$ building blocks

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Figure S1. Experimental and calculated XRD patterns of the $Li_6Rb_5B_{11}O_{22}$.

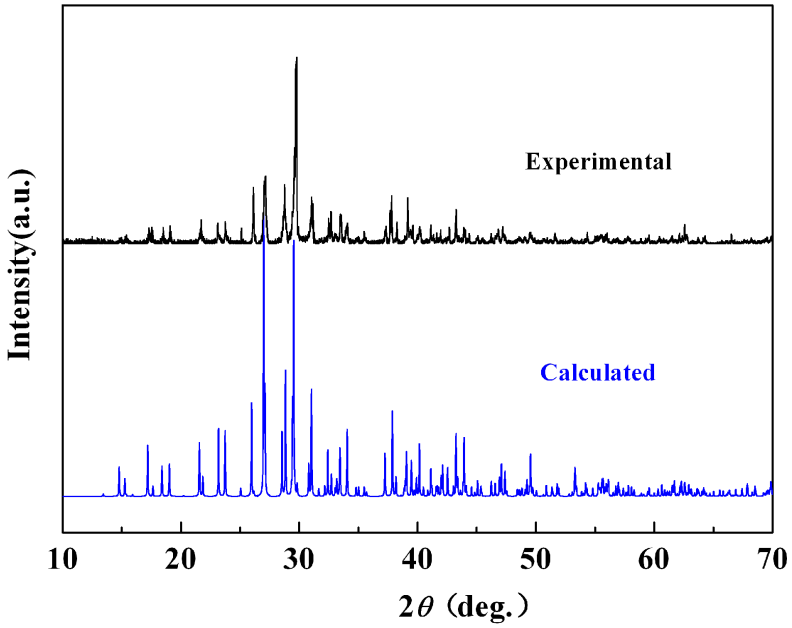


Figure S2. DTA curve of $Li_6Rb_5B_{11}O_{22}$.

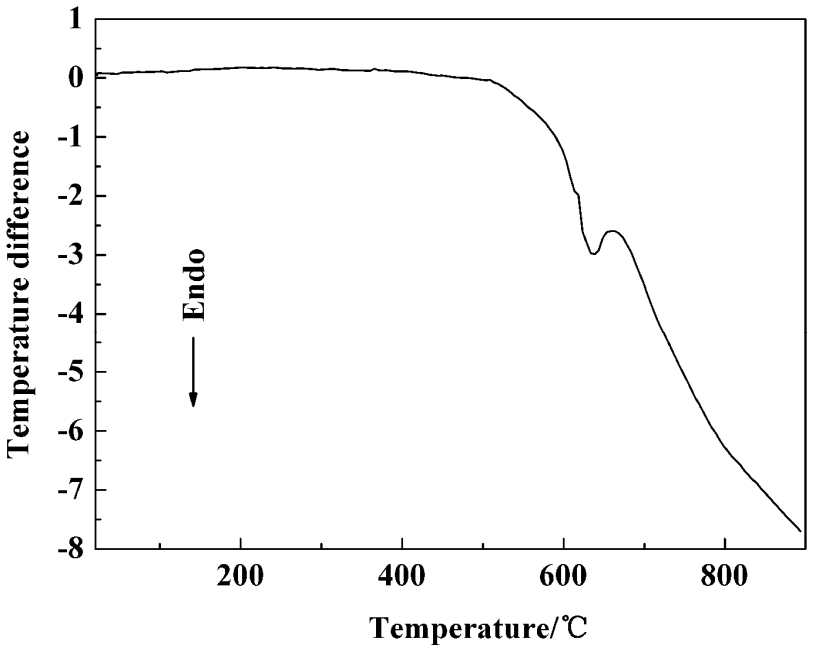


Figure S3. Powder XRD patterns of the $Li_6Rb_5B_{11}O_{22}$ samples before and after melting, respectively.

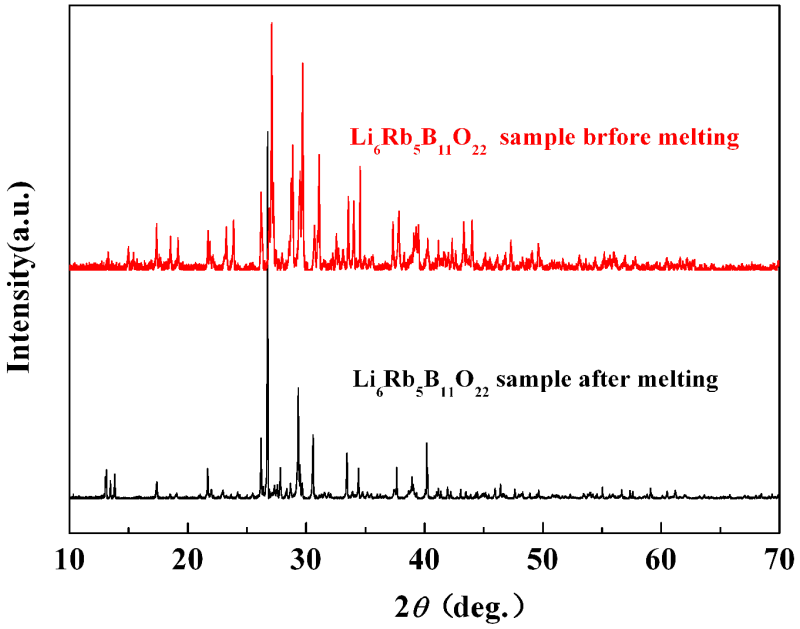


Figure S4. $Rb(1)O_9$, $Rb(2)O_9$ and $Rb(3)O_{10}$ polyhedra are interconnected via sharing oxygen atoms into a 3D framework. (orange, Rb; red, O)

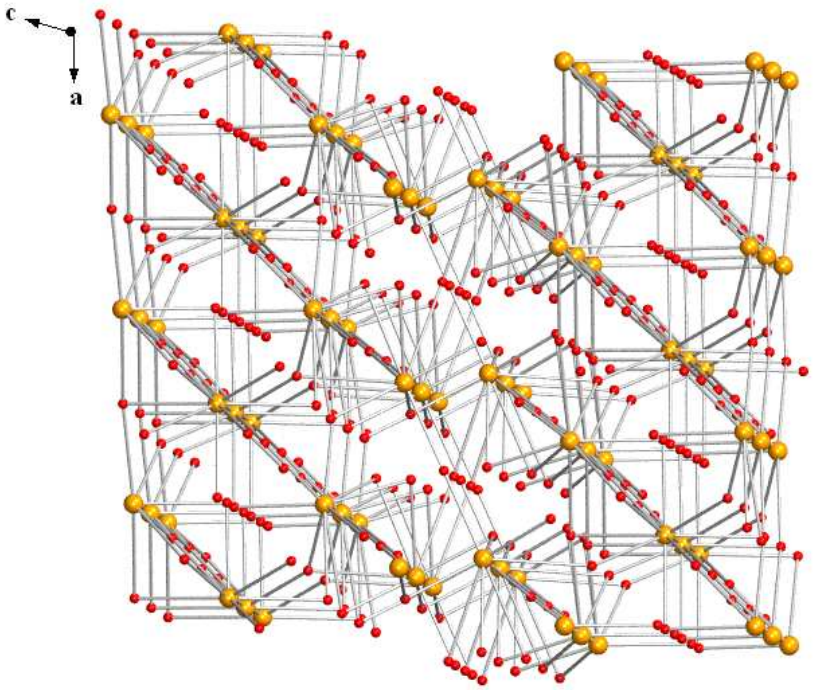
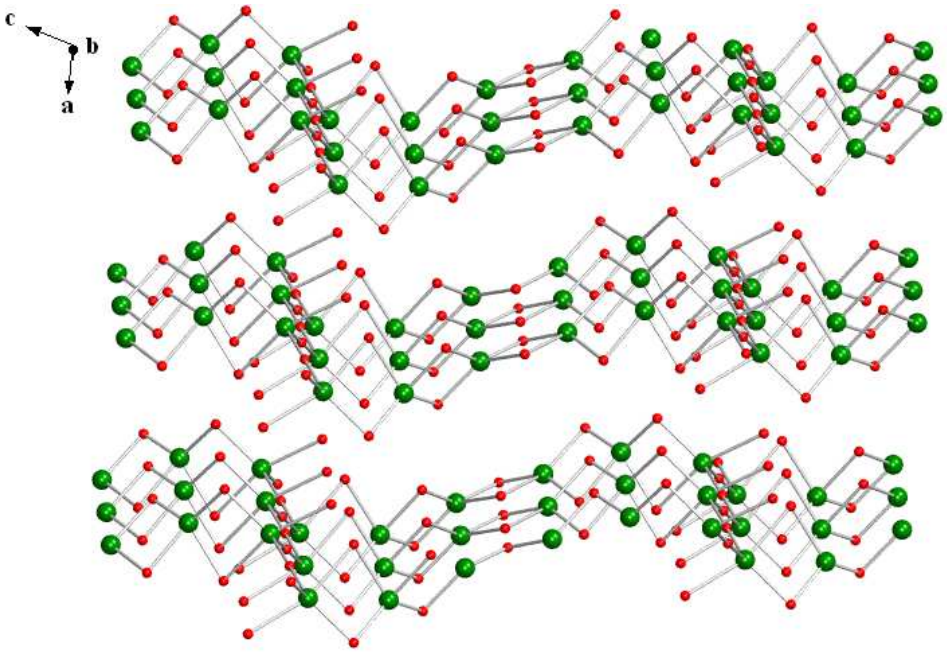
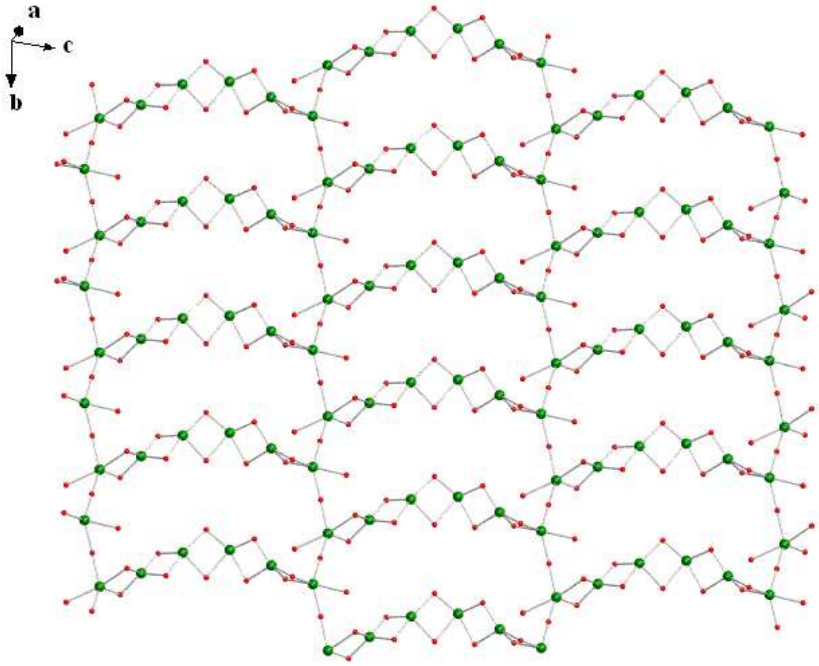


Figure S5 $Li(1)O_4$, $Li(2)O_4$ and $Li(3)O_5$ polyhedra are interconnected via sharing edges into a 2D sheet network. (green, Li; red, O)



(a)



(b)

Figure S6 Infrared (IR) spectroscopy of the $Li_6Rb_5B_{11}O_{22}$ sample.

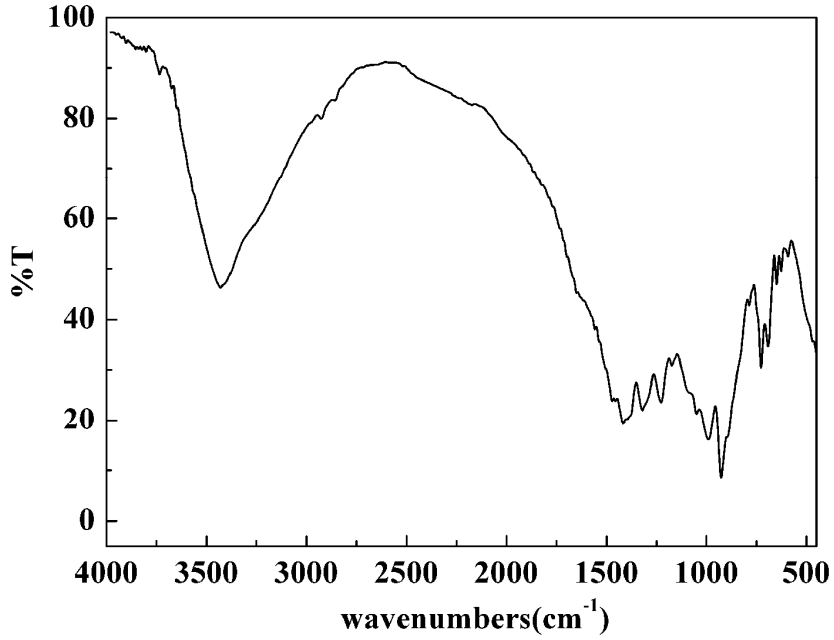


Figure S7. UV-VIS-NIR diffuse-reflectance spectrum of $Li_6Rb_5B_{11}O_{22}$.

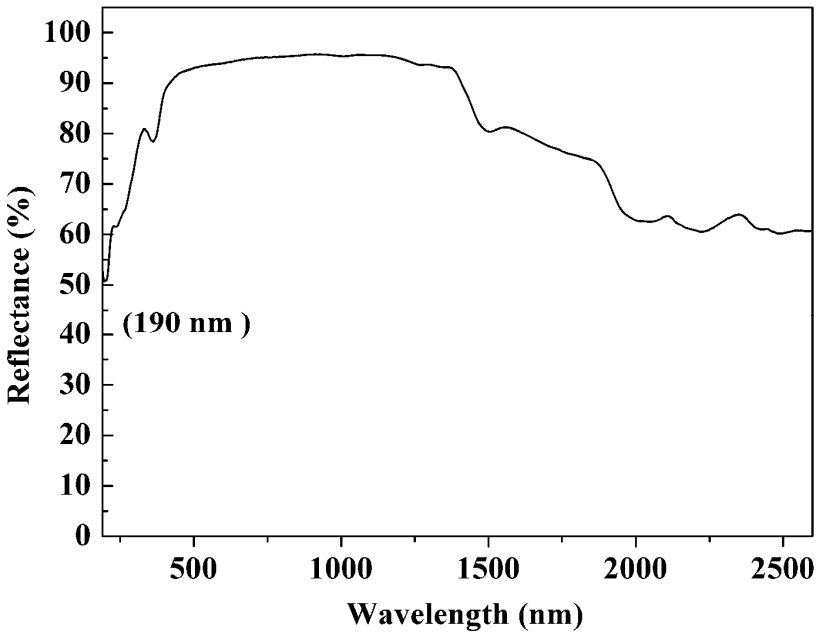


Table S1. Selected bond distances (Å) and angles (deg) for $Li_6Rb_5B_{11}O_{22}$.

Rb(1)-O(8)	2.794(3)	Li(1)-O(10)#7	2.048(9)
Rb(1)-O(12)#1	2.883(3)	Li(1)-O(11)#6	2.123(9)
Rb(1)-O(3)#2	2.954(4)	Li(1)-O(3)	1.878(9)
Rb(1)-O(1)#3	3.109(3)	Li(1)-O(6)#4	1.905(9)
Rb(1)-O(4)	3.123(3)	Li(2)-O(1)	1.868(8)
Rb(1)-O(10)#4	3.239(3)	Li(2)-O(2)#6	2.045(7)
Rb(1)-O(2)	3.344(3)	Li(2)-O(3)	1.831(8)
Rb(1)-O(9)	3.385(3)	Li(2)-O(10)#7	1.989(8)
Rb(1)-O(5)#3	3.438(3)	Li(3)-O(1)#20	1.940(7)
Rb(2)-O(7)#5	2.689(3)	Li(3)-O(2)#17	2.187(9)
Rb(2)-O(5)	2.785(3)	Li(3)-O(4)#18	2.196(9)
Rb(2)-O(6)	2.9591(4)	Li(3)-O(12)	1.965(9)
Rb(2)-O(3)	3.099(4)	Li(3)-O(12)#17	2.020(9)
Rb(2)-O(8)#6	3.242(3)	B(2)-O(7)	1.470(5)
Rb(2)-O(1)	3.334(3)	B(2)-O(8)	1.476(6)
Rb(2)-O(10)#7	3.373(3)	B(2)-O(11)	1.479(5)
Rb(2)-O(11)#6	3.3823(10)	B(2)-O(10)#4	1.478(6)
Rb(2)-O(7)	3.463(4)	B(3)-O(2)#2	1.494(6)
Rb(3)-O(12)#8	2.931(3)	B(3)-O(5)#3	1.485(6)
Rb(3)-O(12)#9	2.931(3)	B(3)-O(9)	1.460(6)
Rb(3)-O(9)	3.111(3)	B(3)-O(10)	1.461(5)
Rb(3)-O(9)#10	3.111(3)	B(4)-O(3)	1.340(6)
Rb(3)-O(1)#1	3.234(3)	B(4)-O(7)	1.376(5)
Rb(3)-O(1)#2	3.234(3)	B(4)-O(9)#4	1.399(6)

Rb(3)-O(4)#1	3.339(3)	B(5)-O(6)	1.331(10)
Rb(3)-O(4)#2	3.339(3)	B(5)-O(8)	1.398(5)
Rb(3)-O(2)#1	3.358(3)	B(5)-O(8)#14	1.398(5)
Rb(3)-O(2)#2	3.358(3)	B(6)-O(4)#18	1.417(6)
B(1)-O(1)	1.326(6)	B(6)-O(2)	1.395(6)
B(1)-O(4)	1.415(6)	B(6)-O(12)	1.313(6)
B(1)-O(5)	1.371(6)	O(7)#5-Rb(2)-O(5)	147.88(11)
O(8)-Rb(1)-O(12)#1	148.95(9)	O(7)#5-Rb(2)-O(6)	93.44(6)
O(8)-Rb(1)-O(3)#2	82.61(9)	O(5)-Rb(2)-O(6)	87.16(8)
O(12)#1-Rb(1)-O(3)#2	128.44(9)	O(7)#5-Rb(2)-O(3)	105.25(10)
O(8)-Rb(1)-O(1)#3	100.54(8)	O(5)-Rb(2)-O(3)	102.91(9)
O(12)#1-Rb(1)-O(1)#3	67.43(8)	O(6)-Rb(2)-O(3)	117.20(11)
O(3)#2-Rb(1)-O(1)#3	118.37(8)	O(7)#5-Rb(2)-O(8)#6	64.51(8)
O(8)-Rb(1)-O(4)	120.06(9)	O(5)-Rb(2)-O(8)#6	99.13(9)
O(12)#1-Rb(1)-O(4)	67.04(8)	O(6)-Rb(2)-O(8)#6	147.22(9)
O(3)#2-Rb(1)-O(4)	88.55(8)	O(3)-Rb(2)-O(8)#6	92.88(8)
O(1)#3-Rb(1)-O(4)	134.39(7)	O(7)#5-Rb(2)-O(1)	148.86(8)
O(8)-Rb(1)-O(10)#4	46.52(8)	(5)-Rb(2)-O(1)	44.43(8)
O(12)#1-Rb(1)-O(10)#4	103.62(8)	O(6)-Rb(2)-O(1)	117.67(5)
O(3)#2-Rb(1)-O(10)#4	126.58(8)	O(3)-Rb(2)-O(1)	60.79(8)
O(1)#3-Rb(1)-O(10)#4	67.44(8)	O(8)#6-Rb(2)-O(1)	87.41(7)
O(4)-Rb(1)-O(10)#4	126.86(8)	O(7)#5-Rb(2)-O(10)#7	86.04(8)
O(8)-Rb(1)-O(2)	87.62(8)	O(5)-Rb(2)-O(10)#7	100.33(8)
O(12)#1-Rb(1)-O(2)	61.82(8)	O(6)-Rb(2)-O(10)#7	166.70(11)

O(3)#2-Rb(1)-O(2)	166.81(7)	O(3)-Rb(2)-O(10)#7	50.58(8)
O(1)#3-Rb(1)-O(2)	54.80(8)	O(8)#6-Rb(2)-O(10)#7	42.81(7)
O(4)-Rb(1)-O(2)	104.05(7)	O(1)-Rb(2)-O(10)#7	63.42(7)
O(10)#4-Rb(1)-O(2)	41.89(7)	O(7)#5-Rb(2)-O(11)#6	45.52(6)
O(8)-Rb(1)-O(9)	107.66(8)	O(5)-Rb(2)-O(11)#6	137.63(7)
O(12)#1-Rb(1)-O(9)	98.20(8)	O(6)-Rb(2)-O(11)#6	134.37(4)
O(3)#2-Rb(1)-O(9)	43.50(8)	O(3)-Rb(2)-O(11)#6	68.97(9)
O(1)#3-Rb(1)-O(9)	78.90(8)	O(8)#6-Rb(2)-O(11)#6	42.86(8)
O(4)-Rb(1)-O(9)	105.10(8)	O(1)-Rb(2)-O(11)#6	104.69(5)
O(10)#4-Rb(1)-O(9)	127.97(7)	O(10)#7-Rb(2)-O(11)#6	41.35(5)
O(2)-Rb(1)-O(9)	133.40(8)	O(7)#5-Rb(2)-O(7)	101.04(10)
O(8)-Rb(1)-O(5)#3	94.49(8)	O(5)-Rb(2)-O(7)	110.25(9)
O(12)#1-Rb(1)-O(5)#3	93.98(8)	O(6)-Rb(2)-O(7)	76.35(10)
O(3)#2-Rb(1)-O(5)#3	76.36(8)	O(3)-Rb(2)-O(7)	41.69(7)
O(1)#3-Rb(1)-O(5)#3	42.05(8)	O(8)#6-Rb(2)-O(7)	129.35(8)
O(4)-Rb(1)-O(5)#3	140.31(8)	O(1)-Rb(2)-O(7)	86.08(7)
O(10)#4-Rb(1)-O(5)#3	90.50(8)	O(10)#7-Rb(2)-O(7)	90.69(7)
O(2)-Rb(1)-O(5)#3	95.70(8)	O(11)#6-Rb(2)-O(7)	91.11(9)
O(9)-Rb(1)-O(5)#3	40.90(8)	O(1)-B(1)-O(5)	122.9(5)
O(12)#8-Rb(3)-O(12)#9	163.38(12)	O(1)-B(1)-O(4)	121.3(4)
O(12)#8-Rb(3)-O(9)	93.76(8)	O(5)-B(1)-O(4)	115.8(4)
O(12)#9-Rb(3)-O(9)	91.32(8)	O(7)-B(2)-O(8)	108.8(4)
O(12)#8-Rb(3)-O(9)#10	91.32(8)	O(7)-B(2)-O(10)#4	109.1(3)
O(12)#9-Rb(3)-O(9)#10	93.76(8)	O(8)-B(2)-O(10)#4	109.9(4)

O(9)-Rb(3)-O(9)#10	144.30(14)	O(7)-B(2)-O(11)	111.2(3)
O(12)#8-Rb(3)-O(1)#1	101.96(8)	O(8)-B(2)-O(11)	110.2(3)
O(12)#9-Rb(3)-O(1)#1	65.88(8)	O(10)#4-B(2)-O(11)	107.6(4)
O(9)-Rb(3)-O(1)#1	145.27(8)	O(9)-B(3)-O(10)	112.4(4)
O(9)#10-Rb(3)-O(1)#1	66.75(8)	O(9)-B(3)-O(5)#3	108.1(4)
O(12)#8-Rb(3)-O(1)#2	65.88(8)	O(10)-B(3)-O(5)#3	111.9(3)
O(12)#9-Rb(3)-O(1)#2	101.96(8)	O(9)-B(3)-O(2)#2	109.4(3)
O(9)-Rb(3)-O(1)#2	66.75(8)	O(10)-B(3)-O(2)#2	105.6(3)
O(9)#10-Rb(3)-O(1)#2	145.27(8)	O(5)#3-B(3)-O(2)#2	109.2(4)
O(1)#1-Rb(3)-O(1)#2	91.66(11)	O(3)-B(4)-O(7)	120.7(4)
O(12)#8-Rb(3)-O(4)#1	63.61(8)	O(3)-B(4)-O(9)#4	120.9(4)
O(12)#9-Rb(3)-O(4)#1	100.89(8)	O(7)-B(4)-O(9)#4	118.4(4)
O(9)-Rb(3)-O(4)#1	126.97(8)	O(6)-B(5)-O(8)#14	122.1(3)
O(9)#10-Rb(3)-O(4)#1	86.59(8)	O(6)-B(5)-O(8)	122.1(3)
O(1)#1-Rb(3)-O(4)#1	42.59(8)	O(8)#14-B(5)-O(8)	115.8(7)
O(1)#2-Rb(3)-O(4)#1	60.26(7)	O(12)-B(6)-O(2)	120.8(4)
O(12)#8-Rb(3)-O(4)#2	100.89(8)	O(12)-B(6)-O(4)#18	121.3(4)
O(12)#9-Rb(3)-O(4)#2	63.61(8)	O(2)-B(6)-O(4)#18	117.9(4)
O(9)-Rb(3)-O(4)#2	86.59(8)	O(3)-Li(1)-O(6)#4	121.5(5)
O(9)#10-Rb(3)-O(4)#2	126.97(9)	O(3)-Li(1)-O(10)#7	89.9(4)
O(1)#1-Rb(3)-O(4)#2	60.26(7)	O(6)#4-Li(1)-O(10)#7	146.6(5)
O(1)#2-Rb(3)-O(4)#2	42.59(8)	O(3)-Li(1)-O(11)#6	133.5(5)
O(4)#1-Rb(3)-O(4)#2	55.67(10)	O(6)#4-Li(1)-O(11)#6	92.5(3)
O(12)#8-Rb(3)-O(2)#1	61.21(8)	O(10)#7-Li(1)-O(11)#6	69.7(3)

O(12)#9-Rb(3)-O(2)#1	130.96(8)	O(3)-Li(2)-O(1)	123.7(4)
O(9)-Rb(3)-O(2)#1	110.86(8)	O(3)-Li(2)-O(10)#7	93.1(3)
O(9)#10-Rb(3)-O(2)#1	43.54(8)	O(1)-Li(2)-O(10)#7	132.1(4)
O(1)#1-Rb(3)-O(2)#1	103.85(7)	O(3)-Li(2)-O(2)#6	130.4(4)
O(1)#2-Rb(3)-O(2)#1	126.80(7)	O(1)-Li(2)-O(2)#6	99.0(3)
O(4)#1-Rb(3)-O(2)#1	99.17(7)	O(10)#7-Li(2)-O(2)#6	71.4(3)
O(4)#2-Rb(3)-O(2)#1	154.76(7)	O(1)#20-Li(3)-O(12)	117.1(4)
O(12)#8-Rb(3)-O(2)#2	130.96(8)	O(1)#20-Li(3)-O(12)#17	116.2(4)
O(12)#9-Rb(3)-O(2)#2	61.21(8)	O(12)-Li(3)-O(12)#17	126.0(4)
O(9)-Rb(3)-O(2)#2	43.54(8)	O(1)#20-Li(3)-O(2)#17	92.2(3)
O(9)#10-Rb(3)-O(2)#2	110.86(8)	O(12)-Li(3)-O(2)#17	101.7(4)
O(1)#1-Rb(3)-O(2)#2	126.80(7)	O(12)#17-Li(3)-O(2)#17	67.9(3)
O(1)#2-Rb(3)-O(2)#2	103.85(7)	O(1)#20-Li(3)-O(4)#18	105.7(4)
O(4)#1-Rb(3)-O(2)#2	154.76(7)	O(12)-Li(3)-O(4)#18	69.5(3)
O(4)#2-Rb(3)-O(2)#2	99.17(7)	O(12)#17-Li(3)-O(4)#18	103.9(3)
O(2)#1-Rb(3)-O(2)#2	106.04(11)	O(2)#17-Li(3)-O(4)#18	162.1(4)

Note. Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,-z+2	#2 x+1/2,y+1/2,z	#3 x+1/2,y-1/2,z
#4 x-1/2,y-1/2,z	#5 -x+1/2,y+1/2,-z+1	#6 x-1/2,y+1/2,z
#7 x-1,y,z	#8 x,y+1,z	#9 -x+2,y+1,-z+2
#10 -x+2,y,-z+2	#11 x+1/2,y+3/2,z	#12 -x+3/2,y+3/2,-z+2
#13 -x+1,y+1,-z+2	#14 -x+1,y,-z+1	#15 -x+1/2,y-1/2,-z+1
#16 x+1,y,z	#17 -x+3/2,y-1/2,-z+2	#18 x,y-1,z
#19 -x,y,-z+1	#20 -x+1,y-1,-z+2	#21 x-1/2,y-3/2,z

Table S2. Bond valence analysis of the $Li_6Rb_5B_{11}O_{22}$.[a,b]

Atoms	l	s	Atoms	l	s
Rb(1)-O(8)	2.794(3)	0.238	Rb(2)-O(7)#5	2.689(3)	0.316
Rb(1)-O(12)#1	2.883(3)	0.187	Rb(2)-O(5)	2.785(3)	0.244
Rb(1)-O(3)#2	2.954(4)	0.154	Rb(2)-O(6)	2.9591(4)	0.152
Rb(1)-O(1)#3	3.109(3)	0.102	Rb(2)-O(3)	3.099(4)	0.104
Rb(1)-O(4)	3.123(3)	0.098	Rb(2)-O(8)#6	3.242(3)	0.071
Rb(1)-O(10)#4	3.239(3)	0.072	Rb(2)-O(1)	3.334(3)	0.055
Rb(1)-O(2)	3.344(3)	0.054	Rb(2)-O(10)#7	3.373(3)	0.050
Rb(1)-O(9)	3.385(3)	0.048	Rb(2)-O(11)#6	3.3823(10)	0.049
Rb(1)-O(5)#3	3.438(3)	0.042	Rb(2)-O(7)	3.463(4)	0.039
∑s		0.995	∑s		1.08
Rb(3)-O(12)#8	2.931(3)	0.164	Li(1)-O(10)#7	2.048(9)	0.207
Rb(3)-O(12)#9	2.931(3)	0.164	Li(1)-O(11)#6	2.123(9)	0.169
Rb(3)-O(9)	3.111(3)	0.101	Li(1)-O(3)	1.878(9)	0.328
Rb(3)-O(9)#10	3.111(3)	0.101	Li(1)-O(6)#4	1.905(9)	0.305
Rb(3)-O(1)#1	3.234(3)	0.072	∑s		1.009
Rb(3)-O(1)#2	3.234(3)	0.072	Li(2)-O(1)	1.868(8)	0.337
Rb(3)-O(4)#1	3.339(3)	0.055	Li(2)-O(2)#6	2.045(7)	0.209
Rb(3)-O(4)#2	3.339(3)	0.055	Li(2)-O(3)	1.831(8)	0.373
Rb(3)-O(2)#1	3.358(3)	0.052	Li(2)-O(10)#7	1.989(8)	0.243
Rb(3)-O(2)#2	3.358(3)	0.052	∑s		1.162
∑s		0.888	Li(3)-O(1)#20	1.940(7)	0.278
B(1)-O(1)	1.326(6)	1.129	Li(3)-O(2)#17	2.187(9)	0.142

B(1)-O(4)	1.415(6)	0.888	Li(3)-O(4)#18	2.196(9)	0.139
B(1)-O(5)	1.371(6)	1.001	Li(3)-O(12)	1.965(9)	0.260
∑s		3.018	Li(3)-O(12)#17	2.020(9)	0.224
B(2)-O(7)	1.470(5)	0.765	∑s		1.043
B(2)-O(8)	1.476(6)	0.753	B(5)-O(6)	1.331(10)	1.114
B(2)-O(11)	1.479(5)	0.747	B(5)-O(8)	1.398(5)	0.930
B(2)-O(10)#4	1.478(6)	0.749	B(5)-O(8)#14	1.398(5)	0.93
∑s		3.014	∑s		2.974
B(3)-O(2)#2	1.494(6)	0.717	B(6)-O(4)#18	1.417(6)	0.883
B(3)-O(5)#3	1.485(6)	0.735	B(6)-O(2)	1.395(6)	0.937
B(3)-O(9)	1.460(6)	0.786	B(6)-O(12)	1.313(6)	1.17
B(3)-O(10)	1.461(5)	0.784	∑s		2.990
∑s		3.022			
B(4)-O(3)	1.340(6)	1.087			
B(4)-O(7)	1.376(5)	0.987			
B(4)-O(9)#4	1.399(6)	0.927			
∑s		3.001			

[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.