Electronic Supplementary Information

$LiRb_2LaB_2O_6$: a new rare earth borate with MOF-5-like topological structure and short UV cut-off edge

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Table S1. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$), and bond valence sums (BVS).

Atoms	*x*	*y*	*z*	*U*(eq)[b]	BVS
Li1	10561(12)	3443(9)	7549(8)	12(2)	2.21
Rb1	2512(1)	888(1)	9559(1)	21(1)	0.93
Rb2	1845(1)	781(1)	5780(1)	24(1)	0.98
La1	6426(1)	2343(1)	7410(1)	9(1)	2.98
B1	8230(9)	2308(6)	9965(6)	13(1)	2.95
B2	6554(9)	-657(7)	7323(6)	15(1)	2.94
O1	9108(5)	3168(4)	6059(3)	15(1)	2.14
O2	9107(5)	2858(4)	8905(4)	16(1)	1.89
O3	6298(5)	2230(4)	9913(4)	18(1)	1.79
O4	4819(5)	-88(4)	7434(4)	17(1)	2.13
O5	3181(5)	2963(4)	7477(4)	16(1)	2.13
O6	8052(5)	171(4)	7078(4)	21(1)	1.90

[b]*U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond lengths (Å) and angles (deg.) for LB-1.

Li1-O2	1.838(9)
Li1-O1	1.858(9)
Li1-O5#1	1.955(10)
Li1-O6#2	2.000(10)
Rb1-O4	2.911(4)
Rb1-O1#6	2.970(4)
Rb1-O5	2.980(4)
Rb1-O3	3.056(4)
Rb1-O1#7	3.057(4)
Rb1-O2#8	3.193(4)
Rb1-O3#9	3.211(4)
Rb1-O5#10	3.213(4)
Rb2-O4	2.849(4)
Rb2-O5	2.906(4)
Rb2-O2#6	2.957(4)
Rb2-O2#11	3.045(4)
Rb2-O6#12	3.062(4)
Rb2-O1#8	3.077(4)
Rb2-O6#8	3.118(4)
La1-O5	2.427(4)
La1-O6	2.452(4)
La1-O2	2.505(4)
La1-O1	2.525(4)
La1-O3	2.558(4)
La1-O3#14	2.581(4)

La1-O4	2.645(4)
La1-O4#3	2.674(4)
B1-O1#10	1.360(7)
B1-O2	1.370(7)
B1-O3	1.400(7)
B2-O5#6	1.378(7)
B2-O6	1.378(8)
B2-O4	1.379(7)
O2-Li1-O1	104.3(5)
O2-Li1-O5#1	121.2(5)
O1-Li1-O5#1	118.3(5)
O2-Li1-O6#2	114.2(5)
O1-Li1-O6#2	123.8(5)
O5#1-Li1-O6#2	74.0(4)
O4-Rb1-O1#6	77.14(11)
O4-Rb1-O5	66.01(11)
O1#6-Rb(1)-O5	121.67(10)
O4-Rb1-O3	73.00(11)
O1#6-Rb1-O3	139.54(11)
O5-Rb1-O3	68.85(11)
O4-Rb1-O1#7	160.65(11)
O1#6-Rb1-O1#7	93.32(10)
O5-Rb1-O1#7	106.81(10)
O3-Rb1-O1#7	122.53(11)
O4-Rb1-O2#8	119.33(10)
O1#6-Rb1-O2#8	101.18(10)
O5-Rb1-O2#8	64.62(10)

O3-Rb1-O2#8	117.03(11)
O1#7-Rb1-O2#8	45.40(10)
O4-Rb1-O3#9	70.07(10)
O1#6-Rb1-O3#9	44.81(10)
O5-Rb1-O3#9	136.08(10)
O3-Rb1-O3#9	98.60(10)
O1#7-Rb1-O3#9	114.75(10)
O2#8-Rb1-O3#9	144.36(10)
B1#9-Rb1-O3#9	25.20(13)
O4-Rb1-O5#10	136.26(11)
O1#6-Rb1-O5#10	124.37(10)
O5-Rb1-O5#10	113.45(5)
O3-Rb1-O5#10	67.35(10)
O1#7-Rb1-O5#10	62.92(10)
O2#8-Rb1-O5#10	95.18(10)
O3#9-Rb1-O5#10	98.01(10)
O4-Rb2-O5	67.79(11)
O4-Rb2-O2#6	79.82(11)
O5-Rb2-O2#6	136.14(11)
O4-Rb2-O2#11	169.79(11)
O5-Rb2-O2#11	105.26(11)
O2#6-Rb2-O2#11	109.86(9)
O4-Rb2-O6#12	116.54(11)
O5-Rb2-O6#12	141.14(11)
O2#6-Rb2-O6#12	79.52(10)
O2#11-Rb2-O6#12	63.72(10)
O4-Rb2-O1#8	130.87(10)

O5-Rb2-O1#8	66.31(10)
O2#6-Rb2-O1#8	124.90(10)
O2#11-Rb2-O1#8	46.47(10)
O6#12-Rb2-O1#8	109.93(10)
O4-Rb2-O6#8	110.77(11)
O5-Rb2-O6#8	100.14(11)
O2#6-Rb2-O6#8	64.03(11)
O2#11-Rb2-O6#8	77.31(11)
O6#12-Rb2-O6#8	112.15(9)
O1#8-Rb2-O6#8	62.30(10)
O5-La1-O6	133.31(13)
O5-La1-O2	132.48(13)
O6-La1-O2	83.62(14)
O5-La1-O1	133.26(13)
O6-La1-O1	80.13(13)
O2-La1-O1	70.93(12)
O5-La1-O1	86.36(13)
O6-La1-O3	97.10(14)
O2-La1-O3	55.78(12)
O1-La1-O3	126.51(12)
O5-La1-O3#14	87.91(13)
O6-La1-O3#14	90.90(13)
O2-La1-O3#14	125.94(12)
O1-La1-O3#14	55.19(12)
O3-La1-O3#14	172.00(9)
O5-La1-O4	78.37(12)
O6-La1-O4	55.64(12)

O2-La1-O4	120.84(12)
O1-La1-O4	129.26(12)
O3-La1-O4	86.06(12)
O3#14-La1-O4	98.26(13)
O5-La1-O4#3	55.72(12)
O6-La1-O4#3	169.70(12)
O2-La1-O4#3	91.94(13)
O1-La1-O4#3	89.64(12)
O3-La1-O4#3	87.99(13)
O3#14-La1-O4#3	84.17(12)
O4-La1-O4#3	133.99(2)
O1#10-B1-O2	124.5(5)
O1#10-B1-O3	118.0(5)
O2-B1-O3	117.5(5)
O5#6-B2-O6	119.6(5)
O5#6-B2-O4	120.6(5)
O6-B2-O4	119.8(5)

Symmetry transformations used to generate equivalent atoms:

#1 x + 1, y, z #2 – x + 2, y+ 1/2, – z + 3/2 #3 – x +1, y + 1/2, – z + 3/2

#4 x + 1, – y + 1/2, z – 1/2 #5 x + 1, – y + 1/2, z + 1/2 #6 – x + 1, y – 1/2, – z + 3/2

#7 x – 1, – y + 1/2, z + 1/2 #8 x – 1, y, z #9 – x + 1, – y, – z + 2

#10 x, – y + 1/2, z + 1/2 #11 x – 1, – y + 1/2, z – 1/2 #12 – x +1, – y, – z + 1

#13 – x, – y, – z + 1 #14 x, – y + 1/2, z – 1/2 #15 – x + 2, y – 1/2, – z + 3/2

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for LB-1.

Atoms	U11	U22	U33	U23	U13	U12
Li1	13(4)	12(4)	11(4)	0(3)	1(3)	-2(3)
Rb1	26(1)	17(1)	21(1)	-1(1)	8(1)	0(1)
Rb2	28(1)	16(1)	27(1)	-1(1)	-12(1)	1(1)
La1	8(1)	9(1)	11(1)	0(1)	0(1)	0(1)
B1	14(3)	16(3)	11(3)	-4(2)	1(2)	-1(2)
B2	17(3)	15(3)	12(3)	0(2)	-1(2)	2(2)
O1	14(2)	19(2)	11(2)	-2(2)	-3(1)	-3(2)
O2	17(2)	18(2)	14(2)	3(2)	2(2)	-6(2)
O3	15(2)	28(2)	12(2)	0(2)	-1(2)	-4(2)
O4	15(2)	13(2)	24(2)	1(2)	2(2)	2(2)
O5	10(2)	11(2)	28(2)	1(2)	0(2)	2(2)
O6	10(2)	15(2)	37(2)	4(2)	5()	-3(2)

Figure S1. Asymmetric unit of selected symmetry-equivalent atoms in LB-1, showing the linkages and coordination spheres with 50 % thermal ellipsoids and atom labels. Symmetry codes: (#1) x, 1/2 – y, 0.5 + 1/2; (#2) – 1 + x, 1/2 – y, 1/2 + z; (#3) – 1 + x, y, z; (#4) 1 – x, – 1/2 + y, 3/2 – z; (#5) – 1 + x, 1/2 – y; – 1/2 + z; (#6) 1 – x, – y, 2 – z; (#7) x, 1/2 – y, – 0.5 + z; (#8) 1 – x, 1/2 + y, 3/2 – z; (#9) 1 + x, y, z; (#10) 1– x, – y, 1– z; (#11) 2 – x, 1/2 + y, 3/2 – z.

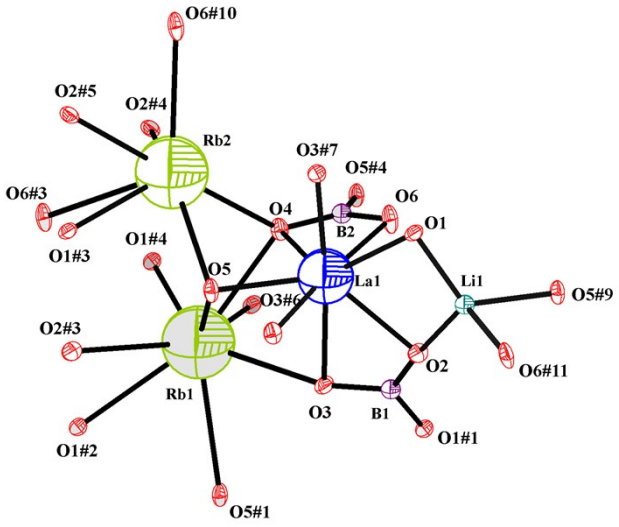

Figure S2. PXRD patterns (left), and pictures of LB-1 in air (upper right) and water (lower right).

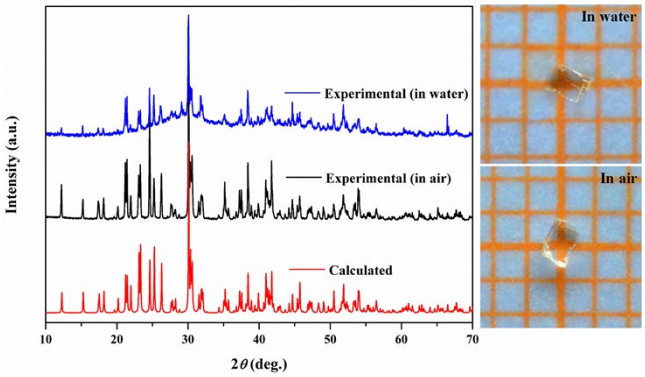

Figure S3. TG-DSC curves for LB-1.

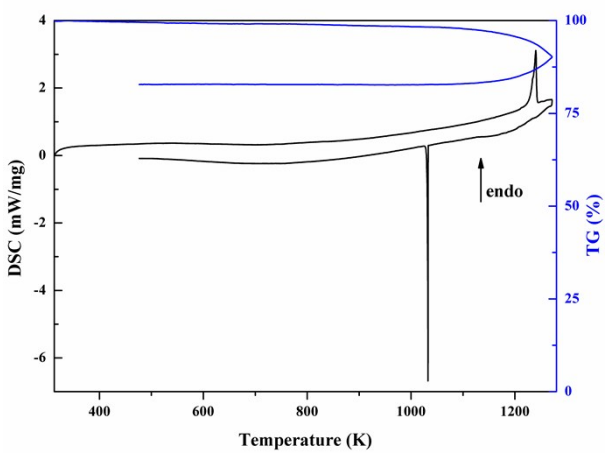

Figure S4. FT-IR spectroscopy for LB-1.

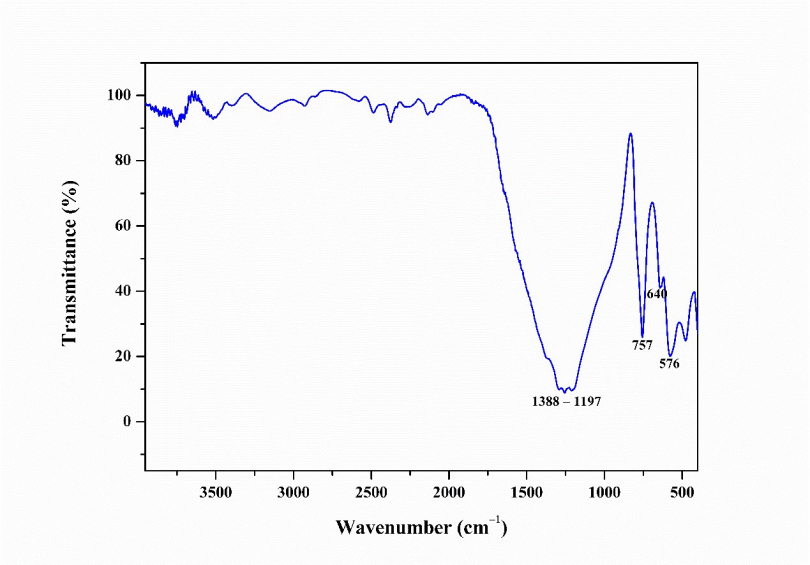

Figure S5. Band structure for LB-1.

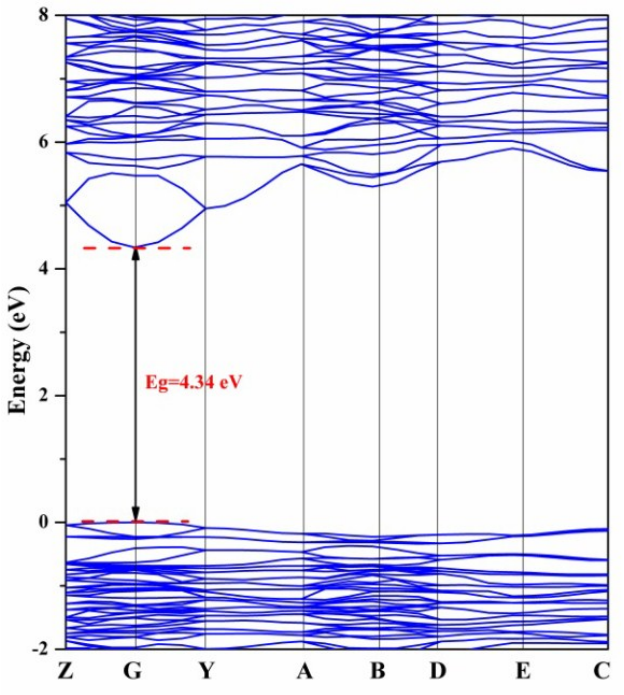

Figure S6. Spatial arrangements of the [BO_3] groups in LB-1 (a), $Na_3La_2(BO_3)_3$ (b), and $Na_3La_9O_3(BO_3)_8$ (c).