Electronic Supplementary Information

$LiCs_2La(BO_3)_2$ and $Li_3K_9La_3(BO_3)_7$: new mixed alkali metal lanthanum borates with three-dimensional open frameworks and short cut-off edges

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CONTENTS

Table S1 Bond lengths [Å] and angles [deg] for (a) $LiCs_2La(BO_3)_2$ and (b) $Li_3K_9La_3(BO_3)_7$.

Table S2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $LiCs_2La(BO_3)_2$ and calculated bond valence sum (BVS).

Table S3 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Li_3K_9La_3(BO_3)_7$ and calculated bond valence sum (BVS).

Table S4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for $LiCs_2La(BO_3)_2$.

Table S5 Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Li_3K_9La_3(BO_3)_7$.

Table S6 Existing complex alkaline and/or alkaline earth lanthanum borates, space group, cation/boron ratio and B-O configuration.

Fig. S1 Experimental and calculated X-ray powder diffraction patterns of (a) $LiCs_2La(BO_3)_2$ and (b) $Li_3K_9La_3(BO_3)_7$.

Fig. S2 The unit cells and asymmetric units of $LiCs_2La(BO_3)_2$ and $Li_3K_9La_3(BO_3)_7$.

Fig. S3 1D infinite $[LiB_2O_6]^{5-}$chain extending along *c* direction.

Fig. S4 The arrangement of the BO_3 units in $LiCs_2La(BO_3)_2$.

Fig. S5 The arrangement of the BO_3 units in $Li_3K_9La_3(BO_3)_7$.

Fig. S6 The La-B-O layered structure along the [100] and [010] directions in $Li_3K_9La_3(BO_3)_7$.

Fig. S7 Isolated $[Li_3O_{10}]$ clusters distributed on the *bc* plane.

Fig. S8 The coordination environment of cations in $Li_3K_9La_3(BO_3)_7$.

Fig. S9 The 1D infinite large channels along the *c* axis in $Li_3K_9La_3(BO_3)_7$.

Fig. S10 The crystal structures of (a)-(d) $LiCs_2La(BO_3)_2$ and (e)-(h) $LiRb_2La(BO_3)_2$.

Fig. S11 The infrared spectra of (a) $LiCs_2La(BO_3)_2$ and (b) $Li_3K_9La_3(BO_3)_7$.

Fig.S12 Band structures of $LiCs_2La(BO_3)_2$. (b) DOS and PDOS for $LiCs_2La(BO_3)_2$.

Fig. S13 The dihedral angles between $B(1)O_3$ and $B(2)O_3$ groups of (a) $Na_3La_2(BO_3)_3$ and (b) $LiCs_2La(BO_3)_2$.

Table S1 Bond lengths [Å] and angles [deg] for (a) $LiCs_2La(BO_3)_2$ and (b) $Li_3K_9La_3(BO_3)_7$.

(a) $LiCs_2La(BO_3)_2$

Li(1)-O(4)#1	1.878(5)	O(2)-Cs(1)-O(4)#10	102.98(7)
Li(1)-O(4)#2	1.878(5)	O(4)#9-Cs(1)-O(4)#10	105.75(5)
Li(1)-O(2)	1.992(8)	O(1)-Cs(1)-O(4)#2	123.44(6)
Li(1)-O(3)#3	2.016(8)	O(2)-Cs(1)-O(4)#2	64.71(7)
Cs(1)-O(1)	2.933(2)	O(4)#9-Cs(1)-O(4)#2	111.38(4)
Cs(1)-O(2)	3.061(2)	O(4)#10-Cs(1)-O(4)#2	44.50(8)
Cs(1)-O(4)#9	3.093(3)	O(1)-Cs(1)-O(3)#11	129.00(8)
Cs(1)-O(4)#10	3.183(2)	O(2)-Cs(1)-O(3)#11	148.03(7)
Cs(1)-O(4)#2	3.213(2)	O(4)#9-Cs(1)-O(3)#11	84.63(7)
Cs(1)-O(3)#11	3.291(14)	O(4)#10-Cs(1)-O(3)#11	63.05(7)
Cs(1)-O(5)	3.451(3)	O(4)#2-Cs(1)-O(3)#11	107.55(7)
Cs(1)-O(5)#2	3.505(15)	O(1)-Cs(1)-O(5)	73.86(7)
Cs(1)-O(2)#13	3.485(17)	O(2)-Cs(1)-O(5)	63.74(5)
La(1)-O(2)	2.448(3)	O(4)#9-Cs(1)-O(5)	139.31(5)
La(1)-O(3)	2.473(3)	O(4)#10-Cs(1)-O(5)	108.86(5)
La(1)-O(4)#6	2.483(2)	O(4)#2-Cs(1)-O(5)	108.18(6)
La(1)-O(4)	2.483(2)	O(3)#11-Cs(1)-O(5)	92.41(6)
La(1)-O(5)	2.6126(9)	O(1)-Cs(1)-O(2)#13	128.15(8)
La(1)-O(5)#6	2.6126(9)	O(2)-Cs(1)-O(2)#13	107.10(4)
La(1)-O(1)	2.682(3)	O(4)#9-Cs(1)-O(2)#13	125.42(6)
La(1)-O(1)#3	2.759(3)	O(4)#10-Cs(1)-O(2)#13	60.31(7)
B(1)-O(4)	1.376(3)	O(4)#2-Cs(1)-O(2)#13	93.62(7)
B(1)-O(4)#14	1.376(3)	O(3)#11-Cs(1)-O(2)#13	41.00(8)
B(1)-O(5)#6	1.377(6)	O(5)-Cs(1)-O(2)#13	59.73(5)
B(2)-O(1)	1.374(6)	O(5)#6-La(1)-O(1)	93.53(3)
B(2)-O(2)#9	1.377(6)	O(5)-La(1)-O(1)	93.53(3)
B(2)-O(3)	1.379(6)	O(4)#6-La(1)-O(1)	124.11(7)
O(4)#1-Li(1)-O(4)#2	101.5(4)	O(3)-La(1)-O(1)	54.75(10)
O(4)#1-Li(1)-O(2)	120.4(3)	O(2)-La(1)-O(3)	135.27(11)
O(4)#2-Li(1)-O(2)	120.4(3)	O(2)-La(1)-O(4)#6	132.03(7)
O(4)#1-Li(1)-O(3)#3	120.8(3)	O(3)-La(1)-O(4)#6	81.13(8)
O(4)#2-Li(1)-O(3)#3	120.8(3)	O(2)-La(1)-O(4)	132.03(7)
O(2)-Li(1)-O(3)#3	72.8(3)	O(3)-La(1)-O(4)	81.13(8)
O(1)-Cs(1)-O(2)	67.21(8)	O(4)#6-La(1)-O(4)	71.74(11)

O(1)-Cs(1)-O(4)#9	76.81(8)	O(2)-La(1)-O(5)	86.03(7)
O(2)-Cs(1)-O(4)#9	127.33(6)	O(3)-La(1)-O(5)	95.82(4)
O(1)-Cs(1)-O(4)#10	167.92(6)	O(2)-La(1)-O(1)#3	54.39(10)
O(4)#6-La(1)-O(5)	55.22(9)	O(3)-La(1)-O(1)#3	170.34(10)
O(4)-La(1)-O(5)	126.54(9)	O(4)#6-La(1)-O(1)#3	91.06(8)
O(2)-La(1)-O(5)#6	86.03(7)	O(4)-La(1)-O(1)#3	91.06(8)
O(3)-La(1)-O(5)#6	95.82(4)	O(5)-La(1)-O(1)#3	84.23(2)
O(4)#6-La(1)-O(5)#6	126.54(9)	O(5)#6-La(1)-O(1)#3	84.23(2)
O(4)-La(1)-O(5)#6	55.22(9)	O(1)-La(1)-O(1)#3	134.90(2)
O(5)-La(1)-O(5)#6	168.36(7)	O(4)-B(1)-O(4)#14	123.3(5)
O(2)-La(1)-O(1)	80.51(10)	O(4)-B(1)-O(5)#6	118.4(2)
O(1)-B(2)-O(2)#9	121.1(4)	O(4)#14-B(1)-O(5)#6	118.4(2)
O(2)#9-B(2)-O(3)	119.4(4)	O(1)-B(2)-O(3)	119.5(4)

Symmetry transformations used to generate equivalent atoms:

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

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

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

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

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

#16 x+1, -y+1/2,z-1/2 #17 x+1,y,-z+1/2 #18 -x+1, y+1/2,z

#19 x+1,y,z

(b) $Li_3K_9La_3(BO_3)_7$			
Li(1)-O(11B)#1	1.732(7)	K(4)-O(5)#4	2.832(2)
Li(1)-O(11B)	1.732(7)	K(4)-O(8)#11	2.849(2)
Li(1)-O(11A)#1	1.935(8)	K(4)-O(5)	2.929(2)
Li(1)-O(11A)	1.935(8)	K(4)-O(3)#12	3.084(2)
Li(1)-O(10)#2	1.944(7)	K(5)-O(2)	2.817(2)
Li(1)-O(10)#3	1.944(7)	K(5)-O(7)	2.860(2)
Li(2)-O(11A)	1.926(8)	K(5)-O(11B)#4	2.953(9)
Li(2)-O(6)#5	1.972(7)	K(5)-O(11B)#14	2.989(10)
Li(2)-O(2)#6	2.030(7)	K(5)-O(9)#14	3.027(3)
Li(2)-O(11B)	2.094(10)	K(5)-O(8)#4	3.083(3)
Li(2)-O11#1	2.102(10)	La(1)-O(7)#4	2.451(2)
Li(2)-O(9)	2.333(9)	La(1)-O(7)	2.451(2)
K(1)-O(8)	2.681(2)	La(1)-O(2)#4	2.511(2)
K(1)-O(8)#4	2.681(2)	La(1)-O(2)	2.511(2)
K(1)-O(7)	2.681(2)	La(1)-O(5)	2.549(2)
K(1)-O(7)#4	2.681(2)	La(1)-O(5)#4	2.549(2)
K(1)-O(4)	2.702(2)	La(1)-O(3)	2.626(2)
K(1)-O(4)#4	2.702(2)	La(1)-O(3)#4	2.626(2)
K(2)-O(9)	2.658(2)	La(2)-O(4)	2.446(2)
K(2)-O(1)	2.709(2)	La(2)-O(9)	2.470(2)
K(2)-O(9)#5	2.779(2)	La(2)-O(8)	2.480(2)
K(2)-O(6)#8	2.795(2)	La(2)-O(6)	2.487(2)
K(2)-O(6)	2.851(2)	La(2)-O(1)	2.5165(5)
K(2)-O(3)#6	2.862(2)	La(2)-O(10)#8	2.526(3)
K(2)-O(5)#6	3.284(2)	La(2)-O(5)#16	2.597(2)
K(3)-O(10)#8	2.797(3)	La(2)-O(3)#7	2.772(2)
K(3)-O(4)	2.798(2)	B(1)-O(4)	1.376(4)
K(3)-O(4)#7	2.810(2)	B(1)-O(7)#7	1.376(4)
K(3)-O(11A)#9	2.820(5)	B(1)-O(3)#7	1.393(4)
K(3)-O(7)#7	2.846(2)	B(2)-O(6)#11	1.364(4)
K(3)-O(2)#4	2.878(2)	B(2)-O(2)	1.380(4)
K(3)-O(7)	2.915(2)	B(2)-O(5)	1.385(4)
K(3)-O(8)#9	2.961(2)	B(3)-O(11B)	1.361(7)
K(3)-O(11B)#9	3.049(7)	B(3)-O(8)	1.369(4)
K(4)-O(3)	2.772(3)	B(3)-O(9)	1.372(4)
K(4)-O(4)#10	2.793(2)	B(3)-O(11A)	1.437(6)

B(4)-O(10)#8	1.362(4)	O(11B)-Li(2)-O(11A)#1	83.6(3)
B(4)-O(10)	1.362(4)	O(11A)-Li(2)-O(6)#5	136.0(4)
B(4)-O(1)	1.369(6)	O(11A)-Li(2)-O(2)#6	150.3(4)
O(11B)#1-Li(1)-O(11B)	124.6(8)	O(6)#5-Li(2)-O(2)#6	73.0(2)
O(11B)#1-Li(1)O(11A)#1	29.0(4)	O(11A)-Li(2)-O(11B)	26.6(3)
O(11B)-Li(1)-O(11A)#1	99.3(5)	O(6)#5-Li(2)-O(11B)	158.4(5)
O(11B)#1-Li(1)-O(11A)	99.3(5)	O(2)#6-Li(2)-O(11B)	123.9(4)
O(11B)-Li(1)-O(11A)	29.0(4)	O(11A)-Li(2)-O(11A)#1	75.9(4)
O(11A)#1-Li(1)-O(11A)	79.7(4)	O(6)#5-Li(2)-O(11A)#1	106.0(4)
O(11B)#1-Li(1)-O(10)#2	116.6(3)	O(2)#6-Li(2)-O(11A)#1	105.3(4)
O(11B)-Li(1)-O(10)#2	106.6(4)	O(11B)-Li(2)-O(11A)#1	83.6(3)
O(11A)#1-Li(1)-O(10)#2	120.03(18)	O(8)-K(1)-O(8)#4	128.50(10)
O(11A)-Li(1)-O(10)#2	135.35(18)	O(8)-K(1)-O(7)	132.83(7)
O(11B)#1-Li(1)-O(10)#3	106.6(4)	O(8)#4-K(1)-O(7)	90.73(7)
O(11B)-Li(1)-O(10)#3	116.6(3)	O(8)-K(1)-O(7)#4	90.73(7)
O(11A)#1-Li(1)-O(10)#3	135.35(18)	O(8)#4-K(1)-O(7)#4	132.83(7)
O(11A)-Li(1)-O(10)#3	120.03(18)	O(7)-K(1)-O(7)#4	74.29(9)
O(10)#2-Li(1)-O(10)#3	75.7(3)	O(8)-K(1)-O(4)	76.09(7)
O(11A)-Li(2)-O(6)#5	136.0(4)	O(8)#4-K(1)-O(4)	84.89(7)
O(11A)-Li(2)-O(2)#6	150.3(4)	O(7)-K(1)-O(4)	83.90(6)
O(6)#5-Li(2)-O(2)#6	73.0(2)	O(7)#4-K(1)-O(4)	135.29(7)
O(11A)-Li(2)-O(11B)	26.6(3)	O(8)-K(1)-O(4)#4	84.89(7)
O(6)#5-Li(2)-O(11B)	158.4(5)	O(8)#4-K(1)-O(4)#4	76.09(7)
O(2)#6-Li(2)-O(11B)	123.9(4)	O(7)-K(1)-O(4)#4	135.29(7)
O(11A)-Li(2)-O(11A)#1	75.9(4)	O(7)#4-K(1)-O(4)#4	83.90(6)
O(6)#5-Li(2)-O(11A)#1	106.0(4)	O(4)-K(1)-O(4)#4	135.43(10)
O(2)#6-Li(2)-O(11A)#1	105.3(4)	O(9)-K(2)-O(1)	74.91(6)
O(11B)-Li(2)-O(11A)#1	83.6(3)	O(9)-K(2)-O(9)#5	98.10(7)
O(11A)-Li(2)-O(6)#5	136.0(4)	O(1)-K(2)-O(9)#5	140.63(7)
O(11A)-Li(2)-O(2)#6	150.3(4)	O(9)-K(2)-O(6)#8	141.23(7)
O(6)#5-Li(2)-O(2)#6	73.0(2)	O(1)-K(2)-O(6)#8	68.00(6)
O(11A)-Li(2)-O(11B)	26.6(3)	O(9)#5-K(2)-O(6)#8	103.29(7)
O(6)#5-Li(2)-O(11B)	158.4(5)	O(9)-K(2)-O(6)	76.90(7)
O(2)#6-Li(2)-O(11B)	123.9(4)	O(1)-K(2)-O(6)	67.19(6)
O(11A)-Li(2)-O(11A)#1	75.9(4)	O(9)#5-K(2)-O(6)	73.48(7)
O(6)#5-Li(2)-O(11A)#1	106.0(4)	O(6)#8-K(2)-O(6)	78.72(7)
O(2)#6-Li(2)-O(11A)#1	105.3(4)	O(9)-K(2)-O(3)#6	114.85(8)

O(1)-K(2)-O(3)#6	84.05(5)	O(7)-K(3)-O(8)#9	125.23(6)
O(9)#5-K(2)-O(3)#6	131.66(7)	O(10)#8-K(3)-O(11B)#9	64.59(15)
O(6)#8-K(2)-O(3)#6	72.72(6)	O(4)-K(3)-O(11B)#9	127.29(19)
O(6)-K(2)-O(3)#6	145.42(6)	O(4)#7-K(3)-O(11B)#9	122.70(13)
O(9)-K(2)-O(5)#6	98.18(7)	O(11A)#9-K(3)-O(11B)#9	17.86(18)
O(1)-K(2)-O(5)#6	144.58(6)	O(7)#7-K(3)-O(11B)#9	102.28(19)
O(9)#5-K(2)-O(5)#6	74.24(6)	O(2)#4-K(3)-O(11B)#9	87.6(2)
O(6)#8-K(2)-O(5)#6	118.51(6)	O(7)-K(3)-O(11B)#9	153.5(2)
O(6)-K(2)-O(5)#6	146.22(6)	O(8)#9-K(3)-O(11B)#9	46.55(12)
O(3)#6-K(2)-O(5)#6	67.16(6)	B(1)#7-K(3)-O(11B)#9	134.94(18)
O(10)#8-K(3)-O(4)	70.50(7)	O(3)-K(4)-O(4)#10	146.99(7)
O(10)#8-K(3)-O(4)#7	167.70(8)	O(3)-K(4)-O(5)#4	78.61(6)
O(4)-K(3)-O(4)#7	98.10(6)	O(4)#10-K(4)-O(5)#4	81.77(6)
O(10)#8-K(3)-O(11A)#9	73.48(11)	O(3)-K(4)-O(8)#11	132.72(7)
O(4)-K(3)-O(11A)#9	142.17(11)	O(4)#10-K(4)-O(8)#11	80.16(6)
O(4)#7-K(3)-O(11A)#9	116.51(11)	O(5)#4-K(4)-O(8)#11	119.00(7)
O(10)#8-K(3)-O(7)#7	89.88(9)	O(3)-K(4)-O(5)	73.62(6)
O(4)-K(3)-O(7)#7	50.80(6)	O(4)#10-K(4)-O(5)	122.45(6)
O(4)#7-K(3)-O(7)#7	79.01(6)	O(5)#4-K(4)-O(5)	68.17(7)
O(11A)#9-K(3)-O(7)#7	118.88(10)	O(8)#11-K(4)-O(5)	74.16(6)
O(10)#8-K(3)-O(2)#4	99.29(10)	O(3)-K(4)-O(3)#12	101.47(6)
O(4)-K(3)-O(2)#4	126.44(7)	O(4)#10-K(4)-O(3)#12	47.32(6)
O(4)#7-K(3)-O(2)#4	91.20(6)	O(5)#4-K(4)-O(3)#12	74.56(6)
O(11A)#9-K(3)-O(2)#4	70.42(10)	O(8)#11-K(4)-O(3)#12	124.95(7)
O(7)#7-K(3)-O(2)#4	168.75(6)	O(5)-K(4)-O(3)#12	142.67(6)
O(10)#8-K(3)-O(7)	128.58(8)	O(4)#10-K(4)-O(6)#7	121.34(6)
O(4)-K(3)-O(7)	78.06(6)	O(5)#4-K(4)-O(6)#7	141.20(6)
O(4)#7-K(3)-O(7)	50.00(6)	O(8)#11-K(4)-O(6)#7	96.80(6)
O(11A)#9-K(3)-O(7)	135.79(10)	O(5)-K(4)-O(6)#7	112.29(6)
O(7)#7-K(3)-O(7)	100.72(6)	O(3)#12-K(4)-O(6)#7	97.89(6)
O(2)#4-K(3)-O(7)	68.45(6)	O(2)-K(5)-O(7)	75.65(6)
O(10)#8-K(3)-O(8)#9	105.96(8)	O(2)-K(5)-O(11B)#4	169.17(13)
O(4)-K(3)-O(8)#9	132.14(7)	O(7)-K(5)-O(11B)#4	104.34(17)
O(4)#7-K(3)-O(8)#9	77.96(7)	O(2)-K(5)-O(11B)#14	77.57(16)
O(11A)#9-K(3)-O(8)#9	49.99(11)	O(7)-K(5)-O(11B)#14	153.14(16)
O(7)#7-K(3)-O(8)#9	82.11(6)	O(11B)#4-K(5)-O(11B)#14	101.6(3)
O(2)#4-K(3)-O(8)#9	101.41(7)	O(2)-K(5)-O(9)#14	72.62(6)

O(7)-K(5)-O(9)#14	126.23(7)	O(7)-La(1)-O(3)	55.84(7)
O(11B)#4-K(5)-O(9)#14	114.51(16)	O(2)#4-La(1)-O(3)	91.38(7)
O(11B)#14-K(5)-O(9)#14	44.74(15)	O(2)-La(1)-O(3)	90.02(7)
O(2)-K(5)-O(8)#4	123.98(7)	O(5)-La(1)-O(3)	82.66(7)
O(7)-K(5)-O(8)#4	79.79(6)	O(5)#4-La(1)-O(3)	86.61(7)
O(11B)#4-K(5)-O(8)#4	46.31(15)	O(7)#4-La(1)-O(3)#4	55.84(7)
O(11B)#14-K(5)-O(8)#4	114.27(16)	O(7)-La(1)-O(3)#4	137.97(7)
O(9)#14-K(5)-O(8)#4	153.67(6)	O(2)#4-La(1)-O(3)#4	90.02(7)
O(2)-K(5)-O(10)#7	135.04(7)	O(2)-La(1)-O(3)#4	91.38(7)
O(7)-K(5)-O(10)#7	118.12(7)	O(5)-La(1)-O(3)#4	86.61(7)
O(11B)#4-K(5)-O(10)#7	54.79(14)	O(5)#4-La(1)-O(3)#4	82.66(7)
O(11B)#14-K(5)-O(10)#7	82.94(13)	O(3)-La(1)-O(3)#4	166.12(10)
O(9)#14-K(5)-O(10)#7	65.11(7)	O(4)-La(2)-O(9)	140.76(7)
O(8)#4-K(5)-O(10)#7	100.95(6)	O(4)-La(2)-O(8)	84.67(7)
O(2)-K(5)-O(10)#15	87.50(8)	O(9)-La(2)-O(8)	57.25(7)
O(7)-K(5)-O(10)#15	121.81(7)	O(4)-La(2)-O(6)	127.36(7)
O(11B)#4-K(5)-O(10)#15	83.36(14)	O(9)-La(2)-O(6)	87.53(7)
O(11B)#14-K(5)-O(10)#15	54.47(14)	O(8)-La(2)-O(6)	127.88(7)
O(9)#14-K(5)-O(10)#15	99.01(7)	O(4)-La(2)-O(1)	120.13(7)
O(8)#4-K(5)-O(10)#15	64.67(6)	O(9)-La(2)-O(1)	81.79(6)
O(10)#7-K(5)-O(10)#15	112.99(9)	O(8)-La(2)-O(1)	126.91(7)
O(7)#4-La(1)-O(7)	82.69(10)	O(6)-La(2)-O(1)	75.95(8)
O(7)#4-La(1)-O(2)#4	89.13(7)	O(4)-La(2)-O(10)#8	80.97(9)
O(7)#4-La(1)-O(2)#4	89.13(7)	O(9)-La(2)-O(10)#8	88.07(11)
O(7)-La(1)-O(2)#4	82.09(7)	O(8)-La(2)-O(10)#8	88.13(11)
O(7)#4-La(1)-O(2)	82.09(7)	O(6)-La(2)-O(10)#8	131.48(8)
O(7)-La(1)-O(2)	89.13(7)	O(1)-La(2)-O(10)#8	55.60(9)
O(2)#4-La(1)-O(2)	168.33(10)	O(4)-La(2)-O(5)#16	93.72(7)
O(7)-La(1)-O(5)	127.02(7)	O(9)-La(2)-O(5)#16	93.14(7)
O(2)#4-La(1)-O(5)	135.10(7)	O(8)-La(2)-O(5)#16	86.63(7)
O(2)-La(1)-O(5)	56.56(7)	O(6)-La(2)-O(5)#16	55.63(7)
O(7)#4-La(1)-O(5)#4	127.02(7)	O(1)-La(2)-O(5)#16	131.53(8)
O(7)-La(1)-O(5)#4	124.03(7)	O(10)#8-La(2)-O(5)#16	172.87(8)
O(2)#4-La(1)-O(5)#4	56.56(7)	O(4)-La(2)-O(3)#7	53.68(7)
O(2)-La(1)-O(5)#4	135.10(7)	O(9)-La(2)-O(3)#7	165.55(7)
O(5)-La(1)-O(5)#4	78.63(9)	O(8)-La(2)-O(3)#7	136.28(7)
O(7)#4-La(1)-O(3)	137.97(7)	O(6)-La(2)-O(3)#7	79.07(7)

O(1)-La(2)-O(3)#7	89.64(5)	O(11B)-B(3)-O(8)	121.1(4)
O(10)#8-La(2)-O(3)#7	96.69(11)	O(11B)-B(3)-O(9)	113.9(4)
O(5)#16-La(2)-O(3)#7	83.83(7)	O(8)-B(3)-O(9)	119.8(3)
O(4)-B(1)-O(7)#7	123.2(3)	O(8)-B(3)-O(11A)	121.3(3)
O(4)-B(1)-O(3)#7	118.1(3)	O(9)-B(3)-O(11A)	116.3(3)
O(7)#7-B(1)-O(3)#7	118.7(3)	O(10)#8-B(4)-O(10)	122.3(5)
O(6)#11-B(2)-O(2)	120.3(3)	O(10)#8-B(4)-O(1)	118.9(2)
O(6)#11-B(2)-O(5)	119.5(3)	O(10)-B(4)-O(1)	118.9(2)
O(2)-B(2)-O(5)	120.2(3)		

Symmetry transformations used to generate equivalent atoms:

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

#3 -x+1,-y+2,-z+1 #4 -x,y,-z+1/2

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

#7 -x,-y+2,-z #8 -x+1, y,-z+1/2

#9 x,-y+2,z-1/2 #10 x,y-1,z

#11 -x,y-1,-z+1/2 #12 -x,-y+1,-z

#13 x,-y+1,z-1/2 #14 x-1,-y+2,z-1/2

#15 x-1,y,z #16 -x,y+1,-z+1/2

#17 x,y+1,z #18 x,-y+1,z+1/2

#19 x+1,y,z

Table S2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $LiCs_2La(BO_3)_2$ and calculated bond valence sum (BVS).

	x/*a*	y/*b*	z/*c*	U(eq)	BVS
Li(1)	3899(1)	12500	2500	14(2)	1.124
Cs(1)	5887(1)	771(1)	4461(1)	22(1)	1.091
La(1)	6426(1)	2265(1)	2500	10(1)	2.847
B(1)	8149(8)	2500	0	13(1)	2.952
B(2)	6566(7)	-702(5)	2500	12(1)	2.954
O(1)	4844(4)	-147(3)	2500	17(1)	1.697
O(2)	3199(4)	2937(3)	2500	15(1)	1.901
O(3)	8085(5)	116(3)	2500	21(1)	1.741
O(4)	9046(3)	2895(2)	1101(2)	16(1)	2.148
O(5)	6261(5)	2500	5000	19(1)	1.707

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

Table S3 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Li_3K_9La_3(BO_3)_7$.

	S.O.F	x/*b*	y/*c*	z/*c*	U(eq)	BVS
Li(1)	1	5000	10636(8)	7500	23(2)	1.320
Li(2)	1	5841(7)	12907(6)	7044(8)	44(2)	0.894
K(1)	1	771(1)	4461(1)	22(1)	1.091	1.361
K(2)	1	6098(1)	14581(1)	4441(1)	21(1)	1.119
K(3)	1	1722(1)	9286(1)	870(1)	20(1)	1.116
K(4)	1	-934(1)	3917(1)	496(1)	24(1)	0.832
K(5)	1	-3381(1)	9060(1)	531(1)	38(1)	0.789
La(1)	1	0	6892(1)	2500	11(1)	3.049
La(2)	1	2839(1)	12975(1)	2546(1)	13(1)	3.078
B(1)	1	949(3)	12143(3)	-13(3)	14(1)	2.988
B(2)	1	-2363(3)	5805(4)	2466(3)	15(1)	2.958
B(3)	1	3689(4)	12243(4)	5075(3)	22(1)	2.935
B(4)	1	5000	11511(6)	2500	36(2)	3.055
O(1)	1	5000	12852(3)	2500	21(1)	—
O(2)	1	2206(2)	7142(2)	2441(2)	20(1)	—
O(3)	1	1365(2)	6582(2)	37(2)	19(1)	—
O(4)	1	799(2)	11789(2)	976(2)	16(1)	—
O(5)	1	1460(2)	4962(2)	2397(2)	19(1)	—
O(6)	1	3421(2)	15304(2)	2463(2)	19(1)	—
O(7)	1	-694(2)	8694(2)	981(2)	17(1)	—
O(8)	1	2403(2)	11926(2)	4102(2)	23(1)	—
O(9)	1	4494(2)	13052(2)	4847(2)	24(1)	—

O(10)	1	6046(3)	10867(3)	2514(4)	72(1)	__
O(11A)	0.5	4082(5)	12090(4)	6367(5)	13(1)	__
O(11B)	0.5	4407(7)	11424(9)	6070(6)	73(3)	__

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

Table S4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for $LiCs_2La(BO_3)_2$.

	$LiCs_2La(BO_3)_2$					
	U11	U22	U33	U23	U13	U12
Li(1)	9(4)	14(4)	20(4)	0	0	0(3)
Cs(1)	28(1)	14(1)	23(1)	0(1)	11(1)	1(1)
La(1)	8(1)	10(1)	11(1)	0	0	0(1)
B(1)	18(3)	9(2)	12(2)	-2(2)	0	0
B(2)	12(2)	13(2)	11(2)	0	0	-1(2)
O(1)	13(2)	16(2)	21(2)	0	0	5(1)
O(2)	10(2)	11(2)	24(2)	0	0	0(1)
O(3)	14(2)	14(2)	34(2)	0	0	1(1)
O(4)	14(1)	20(1)	13(1)	1(1)	-1(1)	-3(1)
O(5)	13(2)	29(2)	15(2)	3(1)	0	0

Table S5 Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Li_3K_9La_3(BO_3)_7$.

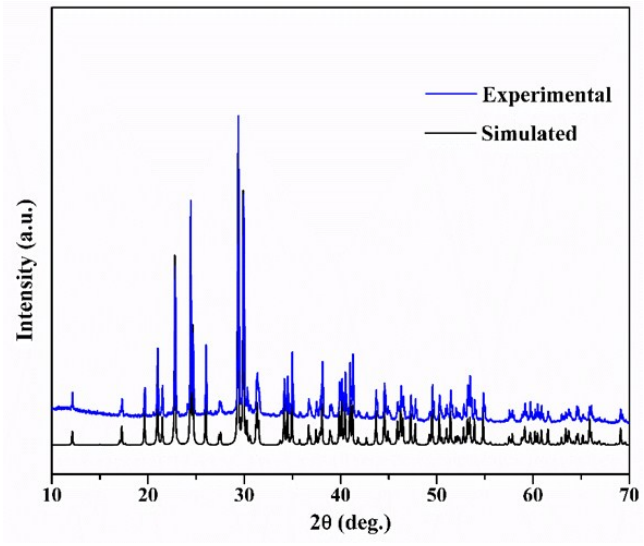
	$Li_3K_9La_3(BO_3)_7$					
	U11	U22	U33	U23	U13	U12
Li(1)	29(4)	20(4)	22(4)	0	15(4)	0
Li(2)	29(4)	31(4)	83(6)	-26(4)	38(4)	-11(3)
K(1)	16(1)	15(1)	14(1)	0	8(1)	0
K(2)	19(1)	23(1)	24(1)	-6(1)	13(1)	-6(1)
K(3)	20(1)	16(1)	22(1)	0(1)	10(1)	-1(1)
K(4)	22(1)	18(1)	31(1)	-1(1)	13(1)	1(1)
K(5)	28(1)	46(1)	41(1)	17(1)	18(1)	7(1)
La(1)	11(1)	10(1)	11(1)	0	6(1)	0
La(2)	11(1)	12(1)	14(1)	-1(1)	6(1)	-2 (1)
B(1)	9(2)	17(2)	13(2)	1(1)	4(1)	0(1)
B(2)	14(2)	18(2)	12(2)	1(1)	7(1)	1(1)
B(3)	18(2)	24(2)	18(2)	4(2)	6(2)	-5(2)
B(4)	20(3)	15(3)	67(5)	0	19(3)	0
O(1)	28(2)	13(2)	29(2)	0	19(2)	0
O(2)	18(1)	14(1)	31(1)	-1(1)	16(1)	-1(1)
O(3)	24(1)	15(1)	16(1)	-1(1)	9(1)	-6(1)
O(4)	18(1)	18(1)	15(1)	15(1)	10(1)	-5(1)
O(5)	17(1)	14(1)	30(1)	3(1)	15(1)	1(1)
O(6)	16(1)	17(1)	31(1)	-4(1)	16(1)	-1(1)
O(7)	3(1)	12(1)	15(1)	-1(1)	10(1)	1(1)
O(8)	16(1)	31(1)	19(1)	0(1)	7(1)	-8(1)

O(9)	18(1)	30(1)	20(1)	1(1)	8(1)	-10(1)
O(10)	40(2)	18(1)	183(4)	28(2)	75(2)	12(1)
O(11A)	16(2)	11(2)	18(2)	-1(2)	13(2)	1(2)
O(11B)	44(4)	101(7)	32(4)	39(4)	-10(3)	-35(4)

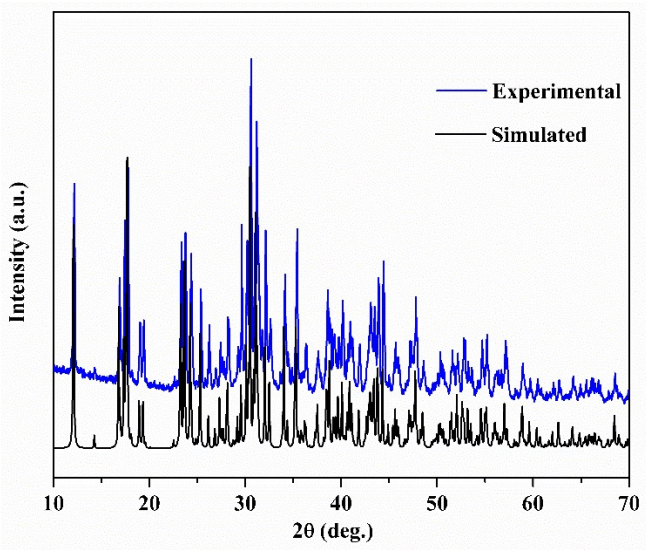
Table S6. Existing complex alkaline and/or alkaline earth lanthanum borates, space group, cation/boron ratio and B-O configuration

	Compounds	Space group	A/B ratio (A=metal ion)	B-O configuration
1	$Li_3K_9La_3(BO_3)_7$	*P2/c* (no.13)	2.14	Isolated BO_3
2	$LiCs_2La(BO_3)_2$	*Pbcm* (no.57)	2	Isolated BO_3
3	$LiRb_2La(BO_3)_2$	$P2_1/c$ (no.14)	2	Isolated BO_3
4	$K_2La_2O(BO_3)_2$	$P2_1/c$ (no.14)	2	Isolated BO_3
5	$Na_3La_2(BO_3)_3$	*Amm*2 (no.38)	1.7	Isolated BO_3
6	$Ca_4LaO(BO_3)_3$	*Cm* (no.8)	1.7	Isolated BO_3
7	$Na_3La_9O_3(BO_3)_8$	*P*-62*m* (no.189)	1.5	Isolated BO_3
8	$LiSr_4La_3(BO_3)_6$	*R*-3 (no.148)	1.3	Isolated BO_3
9	$NaSr_4La_3(BO_3)_6$	*R*-3 (no.148)	1.3	Isolated BO_3
10	$Ba_3La_2(BO_3)_4$	*Pnma* (no.62)	1.25	Isolated BO_3
11	$Ca_3La_2(BO_3)_4$	*Pnma* (no.62)	1.25	Isolated BO_3
12	$Sr_3La_2(BO_3)_4$	$Pna2_1$ (no.3)	1.25	Isolated BO_3
13	$Ca_3La_3(BO_3)_5$	$P6_3mc$ (no.186)	1.2	Isolated BO_3
14	$LaBeB_3O_7$	$Pmn2_1$ (no.31)	0.67	BeB_5O_{18} ring
15	$LaMgB_5O_{10}$	$P2_1/c$ (no.14)	0.5	B_5O_{10} layer
16	$La_2CaB_{10}O_{19}$	*C*2 (no.5)	0.3	B_5O_{12} double-layer

Fig. S1 Experimental and calculated X-ray powder diffraction patterns of (a) $LiCs_2La(BO_3)_2$ and (b) $Li_3K_9La_3(BO_3)_7$.



(a)



(b)

Fig. S2 The unit cells and asymmetric units of $LiCs_2La(BO_3)_2$ and $Li_3K_9La_3(BO_3)_7$

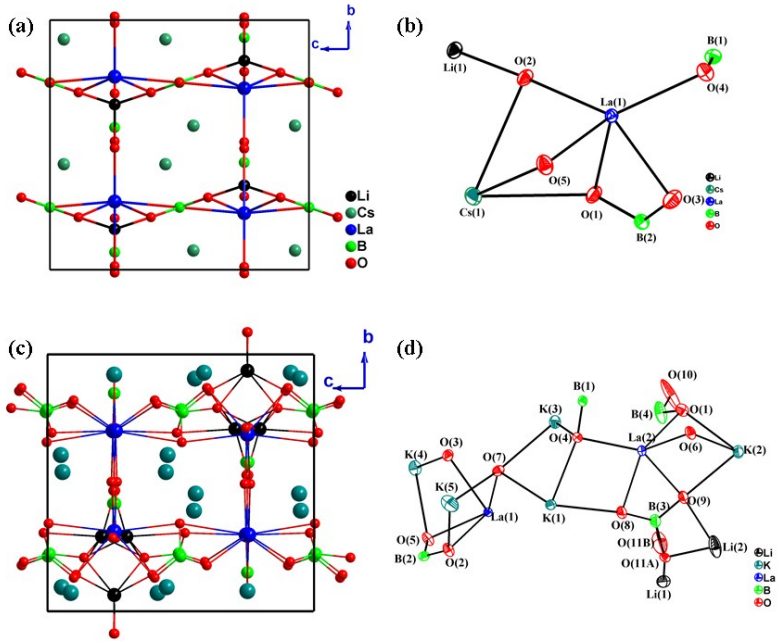


Fig. S3 1D infinite $[LiB_2O_6]^{5-}$chain extending along *c* direction.

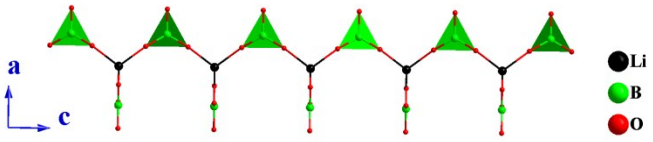


Fig. S4 The arrangement of the BO_3 units in $LiCs_2La(BO_3)_2$.

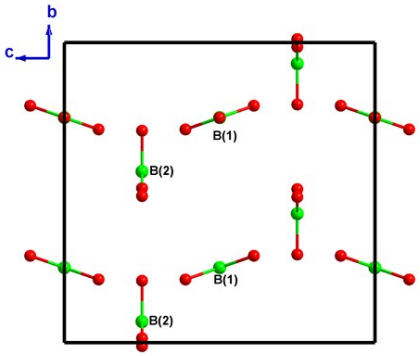


Fig. S5 The arrangement of the BO_3 units in $Li_3K_9La_3(BO_3)_7$.

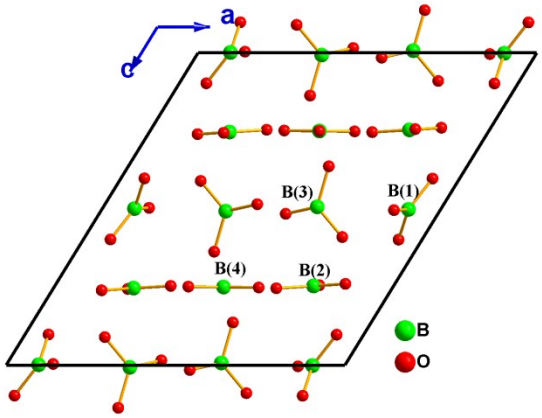


Fig. S6 The La-B-O layered structure along the [100] and [010] directions in $Li_3K_9La_3(BO_3)_7$.

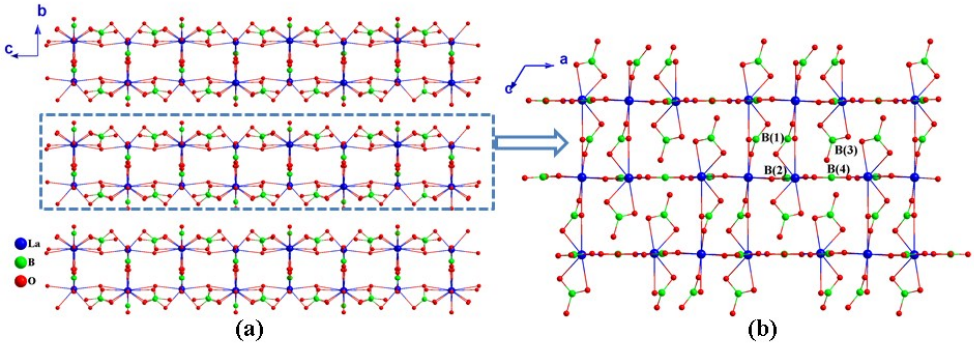


Fig. S7 Isolated $[Li_3O_{10}]$ clusters distributed on the *bc* plane.

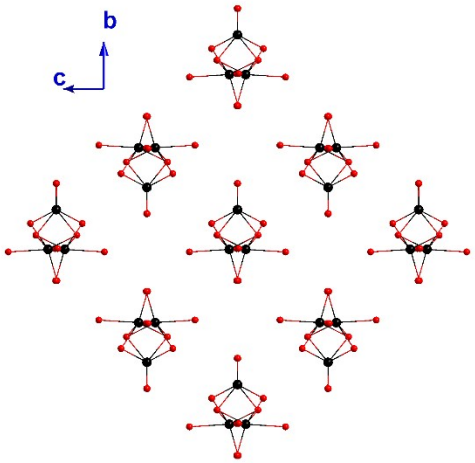


Fig. S8 The coordination environment of cations in $Li_3K_9La_3(BO_3)_7$.

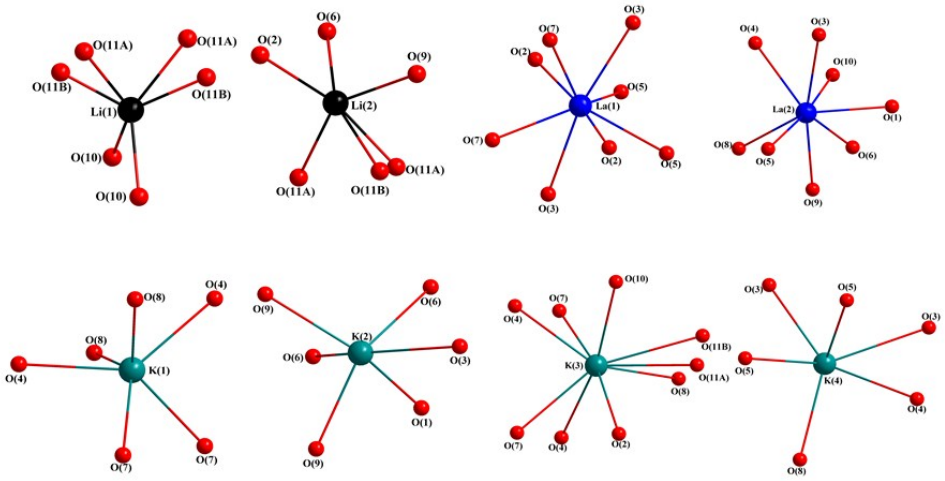


Fig. S9 The 1D infinite large channels along the *c* axis in $Li_3K_9La_3(BO_3)_7$.

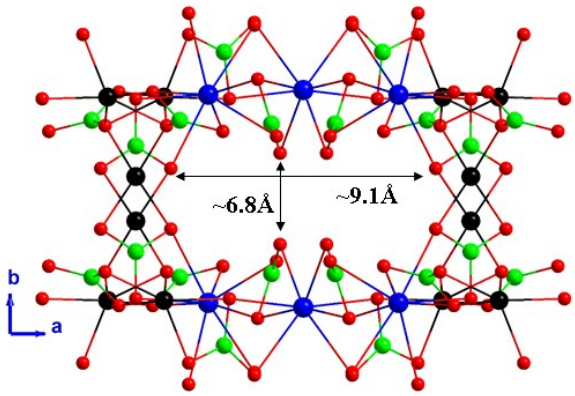


Fig. S10 The crystal structures of (a)-(d) $LiCs_2La(BO_3)_2$ and (e)-(h) $LiRb_2La(BO_3)_2$.

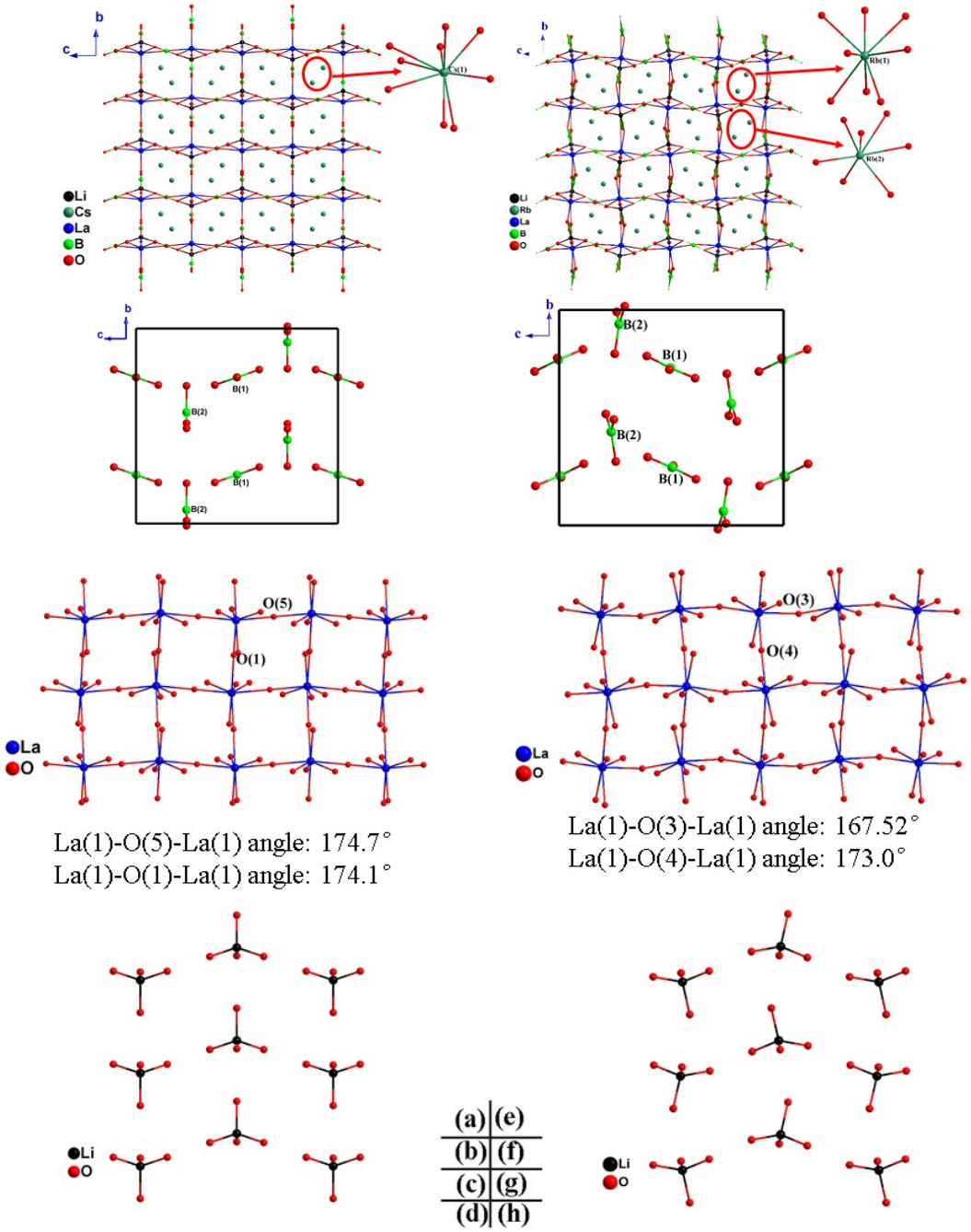


Fig. S11 The infrared spectra of (a) $LiCs_2La(BO_3)_2$ and (b) $Li_3K_9La_3(BO_3)_7$.

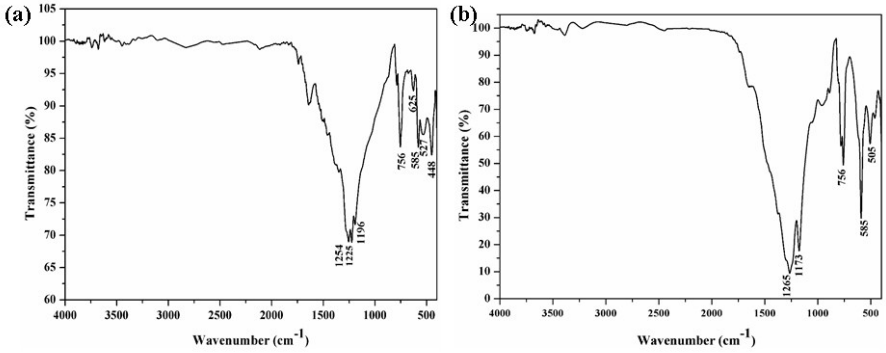


Fig.S12 Band structures of $LiCs_2La(BO_3)_2$. (b) DOS and PDOS for $LiCs_2La(BO_3)_2$.

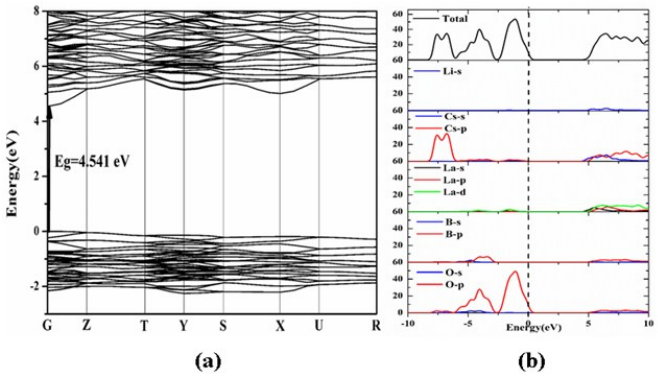


Fig. S13 The dihedral angles between $B(1)O_3$ and $B(2)O_3$ groups of (a) $Na_3La_2(BO_3)_3$ and (b) $LiCs_2La(BO_3)_2$.