Electronic Supplementary Information

Mg assists in modulating the dimensionalities of the anionic frameworks of borates

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Table S1. Atomic coordinates (×10^4), equivalent isotropic displacement parameters (Å^2×10^3) and the Bond Valence Sum (BVS) calculations for $Li_4Mg_3SrB_{12}O_{24}$. [a,b] U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)	BVS
Li(1)/Mg(1)	1632(3)	2332(3)	7522(6)	40(1)	1.25
Mg(2)	0	0	0	7(1)	2.15
Sr(1)	0	0	5000	25(1)	1.95
B(1)	1434(3)	2000(3)	1966(6)	11(1)	2.96
B(2)	3048(3)	2763(3)	4190(6)	10(1)	3.03
O(1)	420(2)	1279(2)	1879(4)	12(1)	1.98
O(2)	1914(2)	2821(2)	584(4)	14(1)	2.04
O(3)	2040(2)	1875(2)	3464(4)	14(1)	1.96
O(4)	2969(2)	2951(2)	6346(4)	11(1)	2.07

[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.

Table S2. Bond lengths (Å) and bond angles (°) of $Li_4Mg_3SrB_{12}O_{24}$.

Chemical bond	Bond length	Chemical bond	Bond length
Li(1)/Mg(1)-O(1)#1	2.012	Sr(1)-O(1)#5	2.631(2)
Li(1)/Mg(1)-O(2)#16	2.089	Sr(1)-O(1)	2.631(3)
Li(1)/Mg(1)-O(2)#14	2.592	Sr(1)-O(3)#1	3.076(2)
Li(1)/Mg(1)-O(3)#5	2.093	Sr(1)-O(3)#3	3.076(2)
Li(1)/Mg(1)-O(4)	1.881	Sr(1)-O(3)#5	3.076(2)
Mg(2)-O(1)	2.072(2)	Sr(1)-O(3)#4	3.076(2)
Mg(2)-O(1)#4	2.072(2)	Sr(1)-O(3)	3.076(2)
Mg(2)-O(1)#6	2.072(2)	Sr(1)-O(3)#2	3.076(2)
Mg(2)-O(1)#7	2.072(2)	B(1)-O(1)	1.341(4)
Mg(2)-O(1)#3	2.072(2)	B(1)-O(2)	1.388(4)
Mg(2)-O(1)#8	2.072(2)	B(1)-O(3)	1.400(4)
Sr(1)-O(1)#1	2.631(3)	B(2)#9-O(2)	1.506(4)

Sr(1)-O(1)#2	2.631(3)	B(2)-O(3)	1.491(4)
Sr(1)-O(1)#3	2.631(2)	B(2)#10-O(4)	1.454(4)
Sr(1)-O(1)#4	2.631(3)	B(2)-O(4)	1.446(4)

Chemical bond	Bond angle	Chemical bond	Bond angle
O(1)#1-Li(1)/Mg(1)-O(2)#16	95.2(2)	O(1)-Sr(1)-O(3)#4	65.76(7)
O(1)#1-Li(1)/Mg(1)-O(2)#14	158.6(2)	O(1)#5-Sr(1)-O(3)#5	47.70(7)
O(1)#1-Li(1)/Mg(1)-O(3)#5	98.95(19)	O(1)#4-Sr(1)-O(3)#2	70.63(7)
O(2)#16-Li(1)/Mg(1)-O(2)#14	97.67(17)	O(1)#2-Sr(1)-O(3)#5	109.37(7)
O(2)#16-Li(1)/Mg(1)-O(3)#5	111.73(19)	O(1)#1-Sr(1)-O(3)#3	114.24(7)
O(3)#5-Li(1)/Mg(1)-O(2)#14	60.34(13)	O(1)#2-Sr(1)-O(3)#2	47.70(7)
O(4)-Li(1)/Mg(1)-O(1)#1	104.3(2)	O(1)#1-Sr(1)-O(3)#1	47.70(7)
O(4)-Li(1)/Mg(1)-O(2)#14	89.14(18)	O(1)#4-Sr(1)-O(3)	109.37(7)
O(4)-Li(1)/Mg(1)-O(2)#16	103.8(2)	O(1)#4-Sr(1)-O(3)#1	132.30(7)
O(4)-Li(1)/Mg(1)-O(3)#5	135.1(2)	O(1)#3-Sr(1)-O(3)	65.76(7)
O(1)#7-Mg(2)-O(1)#3	180.00(11)	O(1)#5-Sr(1)-O(3)#1	109.37(7)
O(1)-Mg(2)-O(1)#3	88.78(10)	O(1)-Sr(1)-O(3)	47.70(7)
O(1)#8-Mg(2)-O(1)#4	91.22(10)	O(1)#3-Sr(1)-O(3)#1	70.63(7)
O(1)-Mg(2)-O(1)#4	88.78(10)	O(1)#4-Sr(1)-O(3)#5	114.24(7)
O(1)-Mg(2)-O(1)#6	91.22(10)	O(1)#2-Sr(1)-O(3)#1	65.76(7)
O(1)#7-Mg(2)-O(1)#4	91.22(10)	O(1)#3-Sr(1)-O(3)#5	132.30(7)
O(1)#8-Mg(2)-O(1)#7	88.78(10)	O(1)-Sr(1)-O(3)#1	114.24(7)
O(1)-Mg(2)-O(1)#7	91.22(10)	O(1)-Sr(1)-O(3)#5	70.63(7)
O(1)#8-Mg(2)-O(1)#6	88.78(10)	O(1)#1-Sr(1)-O(3)#4	132.30(7)
O(1)#8-Mg(2)-O(1)#3	91.22(10)	O(1)#4-Sr(1)-O(3)#3	65.76(7)
O(1)#3-Mg(2)-O(1)#6	91.22(10)	O(1)#4-Sr(1)-O(3)#4	47.70(7)
O(1)#3-Mg(2)-O(1)#4	88.78(10)	O(1)#3-Sr(1)-O(3)#3	47.70(7)
O(1)#7-Mg(2)-O(1)#6	88.78(10)	O(1)#5-Sr(1)-O(3)#4	70.63(7)
O(1)#6-Mg(2)-O(1)#4	180.0(2)	O(1)-Sr(1)-O(3)#3	109.37(7)
O(1)#8-Mg(2)-O(1)	180.0	O(1)#3-Sr(1)-O(3)#4	109.37(7)
O(1)#1-Sr(1)-O(1)#4	180.0	O(1)#1-Sr(1)-O(3)	70.63(7)
O(1)#5-Sr(1)-O(1)#2	66.86(8)	O(3)#1-Sr(1)-O(3)#5	109.98(4)
O(1)#5-Sr(1)-O(1)	113.14(8)	O(3)#1-Sr(1)-O(3)	70.02(4)
O(1)#1-Sr(1)-O(1)#5	66.86(8)	O(3)-Sr(1)-O(3)#3	109.98(4)
O(1)#1-Sr(1)-O(1)	113.14(8)	O(3)#4-Sr(1)-O(3)#5	70.02(4)
O(1)#4-Sr(1)-O(1)#5	113.14(8)	O(3)#4-Sr(1)-O(3)	109.98(4)

O(1)#4-Sr(1)-O(1)#2	113.14(8)	O(3)#2-Sr(1)-O(3)#5	109.98(4)
O(1)#1-Sr(1)-O(1)#3	113.14(8)	O(3)#1-Sr(1)-O(3)#4	180.0
O(1)#3-Sr(1)-O(1)#2	113.14(8)	O(3)-Sr(1)-O(3)#5	70.02(4)
O(1)#4-Sr(1)-O(1)#3	66.86(8)	O(3)#1-Sr(1)-O(3)#3	70.02(4)
O(1)#4-Sr(1)-O(1)	66.86(8)	O(3)#2-Sr(1)-O(3)	180.0
O(1)#5-Sr(1)-O(1)#3	180.0	O(3)#2-Sr(1)-O(3)#3	70.02(4)
O(1)#3-Sr(1)-O(1)	66.86(8)	O(3)#1-Sr(1)-O(3)#2	109.98(4)
O(1)#1-Sr(1)-O(1)#2	66.86(8)	O(3)#5-Sr(1)-O(3)#3	180.00(3)
O(1)#2-Sr(1)-O(1)	180.0	O(3)#4-Sr(1)-O(3)#2	70.02(4)
O(1)#3-Sr(1)-O(3)#2	114.24(7)	O(3)#4-Sr(1)-O(3)#3	109.98(4)
O(1)#5-Sr(1)-O(3)#3	132.30(7)	O(1)-B(1)-O(2)	123.4(3)
O(1)#1-Sr(1)-O(3)#2	109.37(7)	O(1)-B(1)-O(3)	117.5(3)
O(1)-Sr(1)-O(3)#2	132.30(7)	O(2)-B(1)-O(3)	119.0(3)
O(1)#2-Sr(1)-O(3)#4	114.24(7)	O(3)-B(2)-O(2)#10	106.1(3)
O(1)#5-Sr(1)-O(3)	114.24(7)	O(4)-B(2)-O(2)#10	109.4(3)
O(1)#5-Sr(1)-O(3)#2	65.76(7)	O(4)#9-B(2)-O(2)#10	111.6(3)
O(1)#2-Sr(1)-O(3)	132.30(7)	O(4)-B(2)-O(3)	109.6(3)
O(1)#2-Sr(1)-O(3)#3	70.63(7)	O(4)#9-B(2)-O(3)	110.5(3)
O(1)#1-Sr(1)-O(3)#5	65.76(7)	O(4)-B(2)-O(4)#9	109.6(3)

Symmetry transformations used to generate equivalent atoms:

#1 y,-x+y,-z+1	#2 -x,-y,-z+1	#3 -x+y,-x,z
#4 -y,x-y,z	#5 x-y,x,-z+1	#6 y,-x+y,-z
#7 x-y,x,-z	#8 -x,-y,-z	#9 -x+y+1/3,-x+2/3,z-1/3
#10 -y+2/3,x-y+1/3,z+1/3	#14 -x+1/3,-y+2/3,-z+2/3	#16 x,y,z+1

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Li_4Mg_3SrB_{12}O_{24}$.

Atom	**U^{11}**	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**
Li(1)/Mg(1)	28(2)	40(2)	44(2)	-7(2)	4(2)	11(2)
Mg(2)	7(1)	7(1)	7(1)	0	0	3(1)
Sr(1)	34(1)	34(1)	7(1)	0	0	17(1)
B(1)	12(2)	10(2)	8(2)	-3(1)	0(1)	4(1)
B(2)	11(2)	11(2)	8(2)	-1(1)	-1(1)	5(1)
O(1)	9(1)	10(1)	15(1)	-3(1)	-2(1)	4(1)
O(2)	11(1)	13(1)	12(1)	1(1)	-2(1)	2(1)
O(3)	10(1)	12(1)	15(1)	2(1)	-3(1)	1(1)

O(4)	10(1)	16(1)	6(1)	0(1)	1(1)	7(1)

Table S4. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and the BVS calculations for $Rb_2Mg_3B_{16}O_{28}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)	BVS
Rb(1A)	7439(5)	4922(15)	924(4)	55(2)	0.75
Rb(1B)	7533(3)	4685(7)	905(3)	26(1)	0.82
Mg(1)	5000	7505(2)	2500	7(1)	1.99
Mg(2)	9988(1)	7536(2)	969(1)	8(1)	1.96
B(1)	5636(2)	9178(6)	4203(4)	8(1)	3.04
B(2)	5836(2)	5902(6)	4187(4)	8(1)	3.07
B(3)	5686(2)	4177(6)	5861(4)	9(1)	3.09
B(4)	6853(2)	5368(6)	3431(4)	11(1)	3.09
B(5)	8127(2)	5171(6)	3368(4)	12(1)	3.08
B(6)	9127(2)	4207(6)	4145(4)	9(1)	3.08
B(7)	9107(2)	5813(6)	2488(4)	10(1)	3.03
B(8)	9111(2)	9245(6)	2436(4)	9(1)	3.00
O(1)	5628(1)	10671(3)	4796(2)	10(1)	2.07
O(2)	5645(1)	9317(3)	3175(2)	9(1)	2.02
O(3)	5574(1)	7541(3)	4646(2)	9(1)	2.02
O(4)	5575(1)	5598(3)	3178(2)	8(1)	1.98
O(5)	5632(1)	4360(4)	4830(2)	10(1)	2.02
O(6)	5678(1)	2541(3)	6295(2)	10(1)	2.03
O(7)	5689(1)	5646(3)	6465(2)	10(1)	2.08
O(8)	6528(1)	6021(4)	4228(2)	13(1)	1.99
O(9)	6589(1)	4518(4)	2622(2)	12(1)	1.96
O(10)	7503(2)	5661(4)	3496(3)	24(1)	2.18
O(11)	8431(1)	4327(4)	4162(2)	15(1)	1.82
O(12)	8415(1)	5654(4)	2504(2)	12(1)	2.04
O(13)	9395(1)	5561(3)	3508(2)	8(1)	1.96
O(14)	9315(1)	7493(3)	2071(2)	9(1)	1.96

Table S5. Selected bond lengths (Å) and angles (°) for $Rb_2Mg_3B_{16}O_{28}$.

Chemical bond	Bond length	Chemical bond	Bond length
Rb(1A)-O(8)#1	2.971(7)	B(1)-O(2)	1.360(5)
Rb(1A)-O(9)	2.908(8)	B(1)-O(3)	1.370(5)
Rb(1A)-O(10)#1	3.219(7)	B(2)-O(3)	1.487(5)
Rb(1A)-O(10)	3.418(7)	B(2)-O(4)	1.437(5)
Rb(1A)-O(10)#2	3.303(12)	B(2)-O(5)	1.501(5)
Rb(1A)-O(11)#1	3.203(8)	B(2)-O(8)	1.453(5)
Rb(1A)-O(12)	2.918(8)	B(3)-O(5)	1.363(5)
Rb(1B)-O(8)#1	3.042(5)	B(3)-O(6)	1.357(5)
Rb(1B)-O(8)#2	3.398(8)	B(3)-O(7)	1.363(5)
Rb(1B)-O(9)	3.042(6)	B(4)-O(8)	1.360(5)
Rb(1B)-O(10)#1	3.167(5)	B(4)-O(9)	1.345(6)
Rb(1B)-O(10)#2	3.135(5)	B(4)-O(10)	1.377(5)
Rb(1B)-O(10)	3.480(6)	B(5)-O(10)	1.374(5)
Rb(1B)-O(11)#1	3.095(5)	B(5)-O(11)	1.358(6)
Rb(1B)-O(12)	2.848(5)	B(5)-O(12)	1.353(5)
Mg(1)-O(2)	2.097(3)	B(6)-O(1)#8	1.471(6)
Mg(1)-O(2)#3	2.097(3)	B(6)-O(6)#9	1.499(5)
Mg(1)-O(4)#3	2.061(3)	B(6)-O(11)	1.464(5)
Mg(1)-O(4)	2.061(3)	B(6)-O(13)	1.442(5)
Mg(1)-O(6)#4	2.156(3)	B(7)-O(2)#2	1.526(5)
Mg(1)-O(6)#1	2.156(3)	B(7)-O(12)	1.454(5)
Mg(2)-O(1)#2	2.137(3)	B(7)-O(13)	1.466(5)
Mg(2)-O(3)#5	2.154(3)	B(7)-O(14)	1.452(5)
Mg(2)-O(5)#6	2.144(3)	B(8)-O(4)#6	1.466(5)
Mg(2)-O(7)#5	2.099(3)	B(8)-O(7)#8	1.491(5)
Mg(2)-O(13)#7	2.073(3)	B(8)-O(9)#6	1.482(5)
Mg(2)-O(14)	2.048(3)	B(8)-O(14)	1.467(5)
B(1)-O(1)	1.367(5)		

Chemical bond	Bond angle	Chemical bond	Bond angle
O(8)#1-Rb(1A)-O(10)	141.5(3)	O(4)#3-Mg(1)-O(4)	91.34(16)
O(8)#1-Rb(1A)-O(10)#1	43.33(11)	O(4)-Mg(1)-O(6)#1	85.13(10)
O(8)#1-Rb(1A)-O(10)#2	87.6(2)	O(4)#3-Mg(1)-O(6)#4	85.13(10)
O(8)#1-Rb(1A)-O(11)#1	85.29(17)	O(4)#3-Mg(1)-O(6)#1	93.52(11)
O(9)-Rb(1A)-O(8)#1	98.9(3)	O(4)-Mg(1)-O(6)#4	93.52(11)

O(9)-Rb(1A)-O(10)	42.97(12)	O(6)#1-Mg(1)-O(6)#4	178.07(16)
O(9)-Rb(1A)-O(10)#1	141.9(3)	O(1)#2-Mg(2)-O(3)#5	87.44(11)
O(9)-Rb(1A)-O(10)#2	74.99(16)	O(1)#2-Mg(2)-O(5)#6	81.08(11)
O(9)-Rb(1A)-O(11)#1	174.8(3)	O(5)#6-Mg(2)-O(3)#5	88.59(12)
O(9)-Rb(1A)-O(12)	84.75(18)	O(7)#5-Mg(2)-O(1)#2	169.18(12)
O(10)#2-Rb(1A)-O(10)	86.07(19)	O(7)#5-Mg(2)-O(3)#5	81.76(11)
O(10)#1-Rb(1A)-O(10)	175.1(3)	O(7)#5-Mg(2)-O(5)#6	98.02(11)
O(10)#1-Rb(1A)-O(10)#2	95.3(3)	O(13)#7-Mg(2)-O(1)#2	92.56(11)
O(11)#1-Rb(1A)-O(10)#2	108.5(4)	O(13)#7-Mg(2)-O(3)#5	83.25(11)
O(11)#1-Rb(1A)-O(10)	132.5(2)	O(13)#7-Mg(2)-O(5)#6	169.89(12)
O(11)#1-Rb(1A)-O(10)#1	42.59(12)	O(13)#7-Mg(2)-O(7)#5	86.73(11)
O(12)-Rb(1A)-O(8)#1	175.0(6)	O(14)-Mg(2)-O(1)#2	84.50(11)
O(12)-Rb(1A)-O(10)#2	90.0(3)	O(14)-Mg(2)-O(3)#5	171.01(14)
O(12)-Rb(1A)-O(10)#1	132.7(4)	O(14)-Mg(2)-O(5)#6	86.25(11)
O(12)-Rb(1A)-O(10)	42.52(11)	O(14)-Mg(2)-O(7)#5	106.24(12)
O(12)-Rb(1A)-O(11)#1	91.3(2)	O(14)-Mg(2)-O(13)#7	101.04(12)
O(8)#1-Rb(1B)-O(8)#2	102.07(15)	O(1)-B(1)-O(3)	120.2(4)
O(8)#1-Rb(1B)-O(10)#1	43.37(9)	O(2)-B(1)-O(1)	120.0(3)
O(8)#1-Rb(1B)-O(10)	135.3(2)	O(2)-B(1)-O(3)	119.5(3)
O(8)#1-Rb(1B)-O(10)#2	89.46(11)	O(3)-B(2)-O(5)	107.6(3)
O(8)#2-Rb(1B)-O(10)	104.44(15)	O(4)-B(2)-O(3)	111.8(3)
O(8)#1-Rb(1B)-O(11)#1	86.02(13)	O(4)-B(2)-O(5)	106.7(3)
O(9)-Rb(1B)-O(8)#2	113.23(14)	O(4)-B(2)-O(8)	113.3(3)
O(9)-Rb(1B)-O(8)#1	94.46(17)	O(8)-B(2)-O(3)	108.1(3)
O(9)-Rb(1B)-O(10)	41.86(10)	O(8)-B(2)-O(5)	109.2(3)
O(9)-Rb(1B)-O(10)#2	75.78(10)	O(6)-B(3)-O(5)	120.5(4)
O(9)-Rb(1B)-O(10)#1	137.82(19)	O(6)-B(3)-O(7)	119.7(4)
O(9)-Rb(1B)-O(11)#1	168.3(2)	O(7)-B(3)-O(5)	119.5(3)
O(10)#1-Rb(1B)-O(8)#2	82.87(16)	O(8)-B(4)-O(10)	114.2(4)
O(10)#2-Rb(1B)-O(8)#2	40.93(10)	O(9)-B(4)-O(8)	125.1(4)
O(10)#1-Rb(1B)-O(10)	172.2(2)	O(9)-B(4)-O(10)	120.7(4)
O(10)#2-Rb(1B)-O(10)	87.67(11)	O(11)-B(5)-O(10)	117.2(4)
O(10)#2-Rb(1B)-O(10)#1	99.80(15)	O(12)-B(5)-O(10)	118.6(4)
O(11)#1-Rb(1B)-O(8)#2	77.97(17)	O(12)-B(5)-O(11)	124.0(4)
O(11)#1-Rb(1B)-O(10)#2	115.9(2)	O(1)#8-B(6)-O(6)#9	109.0(3)

O(11)#1-Rb(1B)-O(10)	134.36(13)	O(11)-B(6)-O(1)#8	107.5(3)
O(11)#1-Rb(1B)-O(10)#1	43.71(10)	O(11)-B(6)-O(6)#9	110.1(3)
O(12)-Rb(1B)-O(8)#1	174.7(3)	O(13)-B(6)-O(1)#8	111.7(3)
O(12)-Rb(1B)-O(8)#2	83.24(18)	O(13)-B(6)-O(6)#9	106.8(3)
O(12)-Rb(1B)-O(9)	83.56(14)	O(13)-B(6)-O(11)	111.7(3)
O(12)-Rb(1B)-O(10)	42.02(9)	O(12)-B(7)-O(2)#2	107.6(3)
O(12)-Rb(1B)-O(10)#1	138.3(2)	O(12)-B(7)-O(13)	111.2(3)
O(12)-Rb(1B)-O(10)#2	94.82(17)	O(13)-B(7)-O(2)#2	106.5(3)
O(12)-Rb(1B)-O(11)#1	94.92(15)	O(14)-B(7)-O(2)#2	108.8(3)
O(2)#3-Mg(1)-O(2)	98.78(16)	O(14)-B(7)-O(12)	112.8(3)
O(2)-Mg(1)-O(6)#4	97.57(11)	O(14)-B(7)-O(13)	109.6(3)
O(2)#3-Mg(1)-O(6)#1	97.57(11)	O(4)#6-B(8)-O(7)#8	111.9(3)
O(2)#3-Mg(1)-O(6)#4	83.69(11)	O(4)#6-B(8)-O(9)#6	109.4(3)
O(2)-Mg(1)-O(6)#1	83.69(11)	O(4)#6-B(8)-O(14)	108.0(3)
O(4)#3-Mg(1)-O(2)#3	84.99(10)	O(9)#6-B(8)-O(7)#8	106.8(3)
O(4)-Mg(1)-O(2)	84.99(10)	O(14)-B(8)-O(7)#8	106.9(3)
O(4)-Mg(1)-O(2)#3	175.56(11)	O(14)-B(8)-O(9)#6	113.9(3)
O(4)#3-Mg(1)-O(2)	175.56(11)		

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z-1/2	#2 -x+3/2,y-1/2,-z+1/2	#3 -x+1,y,-z+1/2
#4 -x+1,-y+1,-z+1	#5 x+1/2,-y+3/2,z-1/2	#6 -x+3/2,y+1/2,-z+1/2
#7 -x+2,y,-z+1/2	#8 -x+3/2,-y+3/2,-z+1	#9 -x+3/2,-y+1/2,-z+1

Table S6. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Rb_2Mg_3B_{16}O_{28}$.

Atom	**U^{11}**	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**
Rb(1A)	26(2)	120(5)	18(1)	-7(2)	-2(1)	8(2)
Rb(1B)	24(1)	39(2)	19(1)	-1(1)	-3(1)	-5(1)
Mg(1)	8(1)	10(1)	6(1)	0	0(1)	0
Mg(2)	10(1)	7(1)	7(1)	1(1)	0(1)	-1(1)
B(1)	10(2)	4(2)	10(2)	-1(2)	-2(2)	0(2)
B(2)	7(2)	11(2)	6(2)	1(2)	-1(2)	2(2)
B(3)	7(2)	12(2)	9(2)	2(2)	0(2)	-1(2)
B(4)	9(2)	13(2)	12(2)	2(2)	0(2)	0(2)
B(5)	7(2)	15(2)	14(2)	-5(2)	2(2)	-1(2)
B(6)	14(2)	5(2)	10(2)	-4(2)	3(2)	1(2)

B(7)	18(3)	9(2)	4(2)	0(2)	4(2)	-2(2)
B(8)	11(2)	7(2)	8(2)	0(2)	1(2)	1(2)
O(1)	15(2)	6(1)	8(2)	1(1)	1(1)	0(1)
O(2)	15(2)	8(1)	5(1)	0(1)	-1(1)	0(1)
O(3)	14(1)	8(1)	7(1)	2(1)	4(1)	2(1)
O(4)	11(1)	7(1)	5(1)	-2(1)	0(1)	0(1)
O(5)	18(2)	8(1)	7(1)	1(1)	-1(1)	-1(1)
O(6)	17(2)	5(1)	9(2)	0(1)	2(1)	-1(1)
O(7)	18(2)	5(1)	8(2)	-1(1)	-1(1)	-2(1)
O(8)	9(1)	21(2)	12(2)	-4(1)	0(1)	-1(1)
O(9)	12(2)	14(1)	12(2)	-3(1)	4(1)	0(1)
O(10)	9(2)	36(2)	28(2)	-5(2)	1(1)	-2(1)
O(11)	10(2)	22(2)	15(2)	3(1)	2(1)	-1(1)
O(12)	10(2)	15(2)	12(2)	0(1)	0(1)	-1(1)
O(13)	10(1)	7(1)	7(1)	-1(1)	-1(1)	1(1)
O(14)	17(2)	4(1)	8(1)	-2(1)	2(1)	-1(1)

Table S7. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) and the BVS calculations for $Cs_2Mg_3B_{16}O_{28}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)	BVS
Cs(1A)	2486(2)	5384(3)	9093(3)	27(1)	1.07
Cs(1B)	2529(1)	4774(2)	9103(2)	39(1)	1.01
Mg(1)	5000	2490(3)	7500	10(1)	1.97
Mg(2)	10(1)	2472(2)	9040(1)	10(1)	1.94
B(1)	4120(3)	5762(7)	7452(4)	10(1)	3.03
B(2)	4163(2)	4113(7)	5819(4)	8(1)	3.08
B(3)	3147(3)	4765(8)	6602(4)	15(1)	3.09
B(4)	1865(2)	4929(8)	6616(4)	15(1)	3.10
B(5)	877(3)	4180(7)	7494(4)	11(1)	3.02
B(6)	866(2)	5806(7)	5840(4)	10(1)	3.09
B(7)	684(2)	9180(7)	5848(4)	11(1)	3.04
B(8)	647(3)	4182(7)	4193(4)	11(1)	3.00

O(1)	4425(2)	4407(4)	6834(2)	9(1)	1.94
O(2)	3429(2)	5535(5)	7416(3)	15(1)	2.04
O(3)	3475(2)	4016(5)	5824(3)	14(1)	2.01
O(4)	2501(2)	4652(6)	6523(3)	30(1)	2.23
O(5)	1570(2)	4336(5)	7457(3)	15(1)	2.05
O(6)	672(2)	2503(4)	7910(2)	10(1)	1.96
O(7)	600(2)	4437(4)	6471(2)	9(1)	1.94
O(8)	1558(2)	5738(5)	5828(3)	15(1)	2.00
O(9)	658(2)	7535(4)	6270(2)	11(1)	2.04
O(10)	678(2)	10643(4)	6450(2)	11(1)	2.06
O(11)	629(2)	9366(4)	4809(2)	11(1)	2.01
O(12)	625(2)	5669(4)	4787(2)	11(1)	2.06
O(13)	642(2)	4322(4)	3158(2)	10(1)	2.02
O(14)	589(2)	2538(4)	4632(2)	10(1)	2.01

Table S8. Selected bond lengths (Å) and angles (°) for $Cs_2Mg_3B_{16}O_{28}$.

Chemical bond	Bond length	Chemical bond	Bond length
Cs(1A)-O(2)	2.992(5)	B(1)-O(1)	1.461(6)
Cs(1A)-O(3)#1	3.410(4)	B(1)-O(2)	1.464(6)
Cs(1A)-O(3)#2	3.100(5)	B(1)-O(6)#1	1.467(6)
Cs(1A)-O(4)	3.430(6)	B(1)-O(10)#3	1.504(6)
Cs(1A)-O(4)#1	3.322(5)	B(2)-O(1)	1.456(6)
Cs(1A)-O(4)#2	3.200(6)	B(2)-O(3)	1.453(6)
Cs(1A)-O(5)	2.981(5)	B(2)-O(11)#13	1.484(6)
Cs(1A)-O(8)#2	3.143(5)	B(2)-O(14)#6	1.478(6)
Cs(1B)-O(2)	2.996(4)	B(3)-O(2)	1.350(7)
Cs(1B)-O(3)#2	3.133(4)	B(3)-O(3)	1.364(7)
Cs(1B)-O(4)#1	3.773(5)	B(3)-O(4)	1.367(6)
Cs(1B)-O(4)#2	3.218(5)	B(4)-O(4)	1.362(6)
Cs(1B)-O(4)	3.399(5)	B(4)-O(5)	1.354(6)
Cs(1B)-O(5)	2.963(4)	B(4)-O(8)	1.360(7)
Cs(1B)-O(8)#3	3.603(4)	B(5)-O(5)	1.465(6)
Cs(1B)-O(8)#2	3.101(4)	B(5)-O(6)	1.447(6)
Mg(1)-O(1)	2.075(4)	B(5)-O(7)	1.473(6)
Mg(1)-O(1)#4	2.075(4)	B(5)-O(13)#2	1.517(6)

Mg(1)-O(9)#5	2.146(3)	B(6)-O(7)	1.444(6)
Mg(1)-O(9)#3	2.146(3)	B(6)-O(8)	1.457(6)
Mg(1)-O(13)#6	2.101(4)	B(6)-O(9)	1.491(6)
Mg(1)-O(13)#7	2.101(4)	B(6)-O(12)	1.475(6)
Mg(2)-O(6)	2.052(4)	B(7)-O(9)	1.362(6)
Mg(2)-O(7)#8	2.070(4)	B(7)-O(10)	1.360(6)
Mg(2)-O(10)#9	2.097(4)	B(7)-O(11)	1.378(6)
Mg(2)-O(11)#2	2.149(4)	B(8)-O(12)	1.369(6)
Mg(2)-O(12)#2	2.140(4)	B(8)-O(13)	1.367(6)
Mg(2)-O(14)#8	2.171(4)	B(8)-O(14)	1.375(6)

Chemical bond	**Bond angle**	**Chemical bond**	**Bond angle**
O(2)-Cs(1A)-O(3)#2	95.26(15)	O(1)#4-Mg(1)-O(13)#6	175.64(15)
O(2)-Cs(1A)-O(3)#1	113.12(13)	O(1)-Mg(1)-O(13)#7	175.64(15)
O(2)-Cs(1A)-O(4)#2	137.82(16)	O(1)-Mg(1)-O(13)#6	84.87(12)
O(2)-Cs(1A)-O(4)#1	76.99(12)	O(1)#4-Mg(1)-O(13)#7	84.87(12)
O(2)-Cs(1A)-O(4)	42.51(10)	O(9)#3-Mg(1)-O(9)#5	178.2(2)
O(2)-Cs(1A)-O(8)#2	166.49(13)	O(13)#6-Mg(1)-O(9)#3	84.47(13)
O(3)#2-Cs(1A)-O(3)#1	104.61(11)	O(13)#7-Mg(1)-O(9)#3	96.74(13)
O(3)#2-Cs(1A)-O(4)#2	42.97(10)	O(13)#6-Mg(1)-O(9)#5	96.74(13)
O(3)#2-Cs(1A)-O(4)#1	91.75(13)	O(13)#7-Mg(1)-O(9)#5	84.47(13)
O(3)#2-Cs(1A)-O(4)	137.27(16)	O(13)#6-Mg(1)-O(13)#7	98.8(2)
O(3)#1-Cs(1A)-O(4)	100.01(13)	O(6)-Mg(2)-O(7)#8	100.43(14)
O(3)#2-Cs(1A)-O(8)#2	85.59(13)	O(6)-Mg(2)-O(10)#9	104.94(14)
O(4)#2-Cs(1A)-O(3)#1	88.45(13)	O(6)-Mg(2)-O(11)#2	86.31(14)
O(4)#1-Cs(1A)-O(3)#1	40.10(9)	O(6)-Mg(2)-O(12)#2	85.02(14)
O(4)#2-Cs(1A)-O(4)#1	104.63(12)	O(6)-Mg(2)-O(14)#8	172.52(15)
O(4)#2-Cs(1A)-O(4)	170.20(8)	O(7)#8-Mg(2)-O(10)#9	86.99(13)
O(4)#1-Cs(1A)-O(4)	85.10(11)	O(7)#8-Mg(2)-O(11)#2	170.63(15)
O(5)-Cs(1A)-O(2)	84.61(14)	O(7)#8-Mg(2)-O(12)#2	92.82(14)
O(5)-Cs(1A)-O(3)#2	173.01(13)	O(7)#8-Mg(2)-O(14)#8	83.13(14)
O(5)-Cs(1A)-O(3)#1	81.79(12)	O(10)#9-Mg(2)-O(11)#2	97.62(14)
O(5)-Cs(1A)-O(4)#1	95.03(13)	O(10)#9-Mg(2)-O(12)#2	169.92(15)
O(5)-Cs(1A)-O(4)	42.10(10)	O(10)#9-Mg(2)-O(14)#8	81.72(14)
O(5)-Cs(1A)-O(4)#2	135.92(17)	O(11)#2-Mg(2)-O(14)#8	89.45(13)
O(5)-Cs(1A)-O(8)#2	92.92(14)	O(12)#2-Mg(2)-O(11)#2	81.20(13)

O(8)#2-Cs(1A)-O(3)#1	79.53(12)	O(12)#2-Mg(2)-O(14)#8	88.25(14)
O(8)#2-Cs(1A)-O(4)#2	43.01(10)	O(1)-B(1)-O(2)	110.1(4)
O(8)#2-Cs(1A)-O(4)#1	116.49(13)	O(1)-B(1)-O(6)#1	108.0(4)
O(8)#2-Cs(1A)-O(4)	133.44(15)	O(1)-B(1)-O(10)#3	111.9(4)
O(2)-Cs(1B)-O(3)#2	94.50(11)	O(2)-B(1)-O(6)#1	113.3(4)
O(2)-Cs(1B)-O(4)#1	70.10(10)	O(2)-B(1)-O(10)#3	107.1(4)
O(2)-Cs(1B)-O(4)	42.81(10)	O(6)#1-B(1)-O(10)#3	106.5(4)
O(2)-Cs(1B)-O(4)#2	136.82(13)	O(1)-B(2)-O(11)#13	106.5(4)
O(2)-Cs(1B)-O(8)#3	80.67(10)	O(1)-B(2)-O(14)#6	111.5(4)
O(2)-Cs(1B)-O(8)#2	175.83(12)	O(3)-B(2)-O(1)	111.6(4)
O(3)#2-Cs(1B)-O(4)#1	83.26(10)	O(3)-B(2)-O(11)#13	110.1(4)
O(3)#2-Cs(1B)-O(4)#2	42.62(10)	O(3)-B(2)-O(14)#6	108.5(4)
O(3)#2-Cs(1B)-O(4)	137.19(12)	O(14)#6-B(2)-O(11)#13	108.7(4)
O(3)#2-Cs(1B)-O(8)#3	83.93(10)	O(2)-B(3)-O(3)	123.5(5)
O(4)-Cs(1B)-O(4)#1	78.92(10)	O(2)-B(3)-O(4)	120.9(5)
O(4)#2-Cs(1B)-O(4)	173.49(7)	O(3)-B(3)-O(4)	115.5(5)
O(4)#2-Cs(1B)-O(4)#1	94.87(11)	O(5)-B(4)-O(4)	119.0(5)
O(4)#2-Cs(1B)-O(8)#3	96.07(11)	O(5)-B(4)-O(8)	123.6(4)
O(4)-Cs(1B)-O(8)#3	90.25(11)	O(8)-B(4)-O(4)	117.4(5)
O(5)-Cs(1B)-O(2)	84.86(11)	O(5)-B(5)-O(7)	109.9(4)
O(5)-Cs(1B)-O(3)#2	169.34(12)	O(5)-B(5)-O(13)#2	107.0(4)
O(5)-Cs(1B)-O(4)#2	135.94(13)	O(6)-B(5)-O(5)	112.6(4)
O(5)-Cs(1B)-O(4)#1	86.53(10)	O(6)-B(5)-O(7)	110.2(4)
O(5)-Cs(1B)-O(4)	42.48(10)	O(6)-B(5)-O(13)#2	109.4(4)
O(5)-Cs(1B)-O(8)#2	94.13(12)	O(7)-B(5)-O(13)#2	107.5(4)
O(5)-Cs(1B)-O(8)#3	106.42(11)	O(7)-B(6)-O(8)	112.1(4)
O(8)#2-Cs(1B)-O(3)#2	85.74(11)	O(7)-B(6)-O(9)	106.8(4)
O(8)#2-Cs(1B)-O(4)	136.54(12)	O(7)-B(6)-O(12)	111.1(4)
O(8)#2-Cs(1B)-O(4)#2	43.14(10)	O(8)-B(6)-O(9)	109.5(4)
O(8)#3-Cs(1B)-O(4)#1	146.90(11)	O(8)-B(6)-O(12)	108.6(4)
O(8)#2-Cs(1B)-O(4)#1	105.82(10)	O(12)-B(6)-O(9)	108.6(4)
O(8)#2-Cs(1B)-O(8)#3	103.49(9)	O(9)-B(7)-O(11)	119.7(4)
O(1)#4-Mg(1)-O(1)	91.5(2)	O(10)-B(7)-O(9)	120.1(4)
O(1)#4-Mg(1)-O(9)#3	92.82(13)	O(10)-B(7)-O(11)	119.7(4)
O(1)#4-Mg(1)-O(9)#5	85.89(13)	O(12)-B(8)-O(14)	119.7(4)

O(1)-Mg(1)-O(9)#3	85.89(13)	O(13)-B(8)-O(12)	120.4(4)
O(1)-Mg(1)-O(9)#5	92.82(13)	O(13)-B(8)-O(14)	119.3(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z+1/2	#2 -x+1/2,y+1/2,-z+3/2	#3 -x+1/2,y-1/2,-z+3/2
#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+1/2
#7 -x+1,y,-z+3/2	#8 -x,y-1,-z+3/2	#9 -x,y,-z+3/2
#13 -x,y+1,-z+3/2		

Table S9. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Cs_2Mg_3B_{16}O_{28}$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cs(1A)	27(1)	42(1)	14(1)	-1(1)	-1(1)	-2(1)
Cs(1B)	25(1)	79(1)	13(1)	0(1)	-1(1)	-7(1)
Mg(1)	11(1)	10(1)	9(1)	0	-1(1)	0
Mg(2)	11(1)	9(1)	10(1)	1(1)	-1(1)	0(1)
B(1)	18(3)	10(3)	2(2)	0(2)	-2(2)	2(2)
B(2)	11(2)	10(3)	4(2)	-1(2)	2(2)	0(2)
B(3)	12(2)	18(3)	17(3)	5(2)	1(2)	-4(2)
B(4)	8(2)	21(3)	16(3)	-4(2)	3(2)	1(2)
B(5)	15(3)	9(3)	8(2)	1(2)	-5(2)	0(2)
B(6)	10(2)	11(3)	8(2)	-2(2)	2(2)	0(2)
B(7)	9(2)	11(3)	12(3)	1(2)	-2(2)	1(2)
B(8)	11(2)	13(3)	10(3)	-1(2)	-2(2)	-2(2)
O(1)	11(2)	9(2)	7(2)	-1(1)	-1(1)	2(1)
O(2)	14(2)	19(2)	11(2)	-3(1)	5(1)	-2(1)
O(3)	8(2)	23(2)	13(2)	-2(1)	0(1)	-1(1)
O(4)	9(2)	59(3)	23(2)	-3(2)	1(2)	0(2)
O(5)	10(2)	22(2)	12(2)	0(1)	-3(1)	0(1)
O(6)	15(2)	9(2)	6(2)	1(1)	0(1)	1(1)
O(7)	10(2)	10(2)	8(2)	2(1)	-1(1)	0(1)
O(8)	8(2)	22(2)	14(2)	2(1)	1(1)	-2(1)
O(9)	21(2)	8(2)	5(2)	-1(1)	1(1)	1(1)
O(10)	18(2)	9(2)	5(2)	1(1)	-2(1)	0(1)
O(11)	20(2)	9(2)	5(2)	0(1)	2(1)	-1(1)
O(12)	18(2)	9(2)	5(2)	1(1)	-1(1)	2(1)
O(13)	15(2)	9(2)	7(2)	-1(1)	1(1)	-2(1)

O(14)	17(2)	11(2)	4(1)	0(1)	2(1)	1(1)

Table S10. Basic information on anhydrous alkali and/or alkaline-earth metal Mg-containing borates.

No.	Cation	Compound	Space group	Anion framework dimensions	N_{cation}/N_B
1.	**Mg**	$Mg_3(BO_3)F_3$	$P6_3/m$	0D cluster, $[BO_3]$	3
2.		$Mg_2(BO_3)F$	$Pnam$	0D cluster, $[BO_3]$	2
3.		$Mg_2(BO_3)_{1.14}F_{0.58}$	$Pna2_1$	0D cluster, $[BO_3]$	1.75
4.		$Mg_5(BO_3)_3F$	$Pnma$	0D cluster, $[BO_3]$	1.67
5.		$Mg_5(BO_3)_3F$	$Pna2_1$	0D cluster, $[BO_3]$	1.67
6.		$Mg_3(BO_3)_2$	$Pnnm$	0D cluster, $[BO_3]$	1.5
7.		$Mg_2(B_2O_5)$	$P2_1/c$	0D cluster, $[B_2O_5]$	1
8.		$Mg_2(B_2O_5)$	$P\bar{1}$	0D cluster, $[B_2O_5]$	1
9.		$Mg_3(B_7O_{13}Cl)$	$F\bar{4}3c$	3D network	0.43
10.		$Mg_3(B_7O_{13}Cl)$	$Pca2_1$	3D network	0.43
11.		$MgO(B_2O_3)_2$	$Pbca$	3D network	0.25
12.	**Alkali metal and Mg**	$LiMg(BO_3)$	$C2/c$	0D cluster, $[BO_3]$	2
13.		$NaMgBO_3$	$C2/c$	0D cluster, $[BO_3]$	2
14.		$KMg(BO_3)$	$P2_13$	0D cluster, $[BO_3]$	2
15.		$RbMg(BO_3)$	$P2_13$	0D cluster, $[BO_3]$	2
16.		$Cs_4Mg_4(BO_3)_4$	$P2_1/c$	0D cluster, $[BO_3]$	2
17.		$K_{0.83}Na_{0.17}Mg(BO_3)$	$P2_13$	0D cluster, $[BO_3]$	2
18.		$K_{0.92}Na_{0.08}Mg(BO_3)$	$P2_13$	0D cluster, $[BO_3]$	2
19.		$Li_{0.8}Mg_{2.1}B_2O_5F$	$P2_1/n$	0D cluster, $[B_2O_5]$	1.5
20.		$Rb_{18}Mg_6(B_5O_{10})_3(B_7O_{14})_2F$	$C2/c$	0D cluster, $[B_5O_{10}]$+ $[B_7O_{14}]$	0.83
21.		$Cs_{18}Mg_6(B_5O_{10})_3(B_7O_{14})_2F$	$C2/c$	0D cluster, $[B_5O_{10}]$+ $[B_7O_{14}]$	0.83

22.		$Na_3Mg(B_5O_{10})$	*Pbca*	0D cluster, $[B_5O_{10}]$	0.8
23.		***$Rb_2Mg_3B_{16}O_{28}$**	***C2/c***	**2D bilayer**	**0.31**
24.		***$Cs_2Mg_3B_{16}O_{28}$**	***C2/c***	**2D bilayer**	**0.31**
25.	**Alkaline-earth metal and Mg**	$BaMg(BO_3)F$	*Cc*	0D cluster, $[BO_3]$	2
26.		$BaMgBe_2(BO_3)_2F$	$P\bar{3}c1$	0D cluster, $[BO_3]$	2
27.		$Ba_2Mg(BO_3)_2$	$R\bar{3}m$	0D cluster, $[BO_3]$	1.5
28.		$MgSrB_2O_5$	$P2_1/c$	0D cluster, $[B_2O_5]$	1.5
29.		$Sr_2Mg(BO_3)_2$	*C2/m*	0D cluster, $[BO_3]$	1.5
30.		$CaMg(B_2O_5)$	$Pc2_1b$	0D cluster, $[B_2O_5]$	1
31.		$CaMg(B_2O_5)$	*Pbca*	0D cluster, $[B_2O_5]$	1
32.		$CaMg(B_2O_5)$	$P2_1/c$	0D cluster, $[B_2O_5]$	1
33.		$Sr_8MgB_{18}O_{36}$	$R\bar{3}c$	0D cluster, $[B_{18}O_{36}]$	0.5
34.		$Ba_2MgB_6O_{12}$	$R\bar{3}$	0D cluster, $[B_3O_6]$	0.5
35.		$Ca_{0.88}Mg_{0.12}B_5O_7F_3$	$Cmc2_1$	2D monolayer	0.2
36.		$Ca_{0.9}Mg_{0.1}B_5O_7F_3$	$Cmc2_1$	2D monolayer	0.2
37.		$Ca_{0.92}Mg_{0.08}B_5O_7F_3$	$Cmc2_1$	2D monolayer	0.2
38.		$Ca_{0.925}Mg_{0.075}B_5O_7F_3$	$Cmc2_1$	2D monolayer	0.2
39.		$Ca_{0.93}Mg_{0.07}B_5O_7F_3$	$Cmc2_1$	2D monolayer	0.2
40.		$Ca_{0.94}Mg_{0.06}B_5O_7F_3$	$Cmc2_1$	2D monolayer	0.2
41.	**Alkali, alkaline-earth metal, and Mg**	$Li_{13}(Be_{0.55}Mg_{0.45})Be_6(BO_3)_9$	$P6_3/m$	0D cluster, $[BO_3]$	2.22
42.		$KBa_7Mg_2B_{14}O_{28}F_5$	*C2/c*	0D cluster, $[B_7O_{14}]$	0.71
43.		$NaBa_7Mg_2B_{14}O_{28}F_5$	*C2/c*	0D cluster, $[B_7O_{14}]$	0.71
44.		***$Li_4Mg_3SrB_{12}O_{24}$**	***$R\bar{3}$***	**1D chain**	**0.67**

Note: (1) The title compounds are marked with * and boldfaced style.

(2) The natural mineral and mixed anions structures are not included.

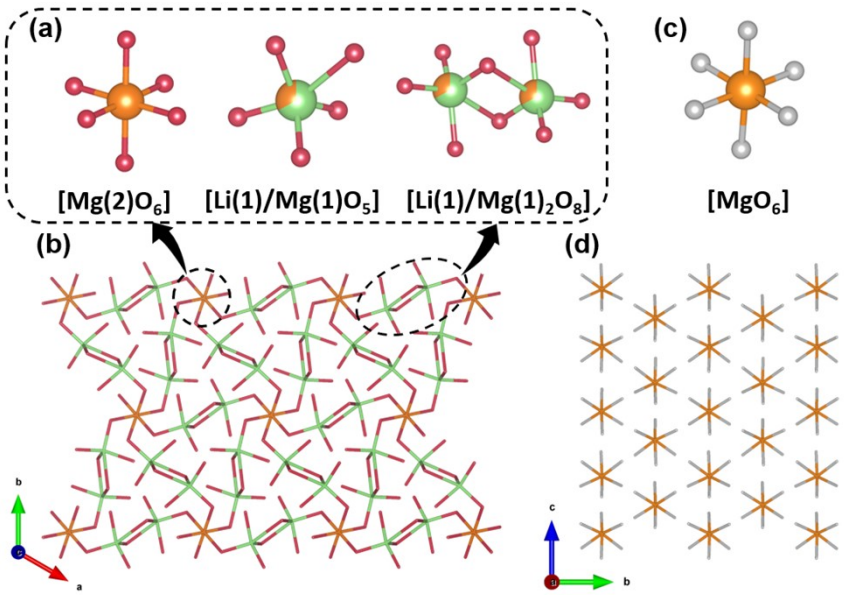

Figure S1. (a) The coordination environments of Mg atoms, and (b) the connections between $[Li(1)/Mg(1)_2O_8]$ dimers and $[Mg(2)O_6]$ polyhedra of $Li_4Mg_3SrB_{12}O_{24}$. (c) the coordination environment of Mg atom, and (d) isolated $[MgO_6]$ polyhedra of $Cs_2Mg_3B_{16}O_{28}$.

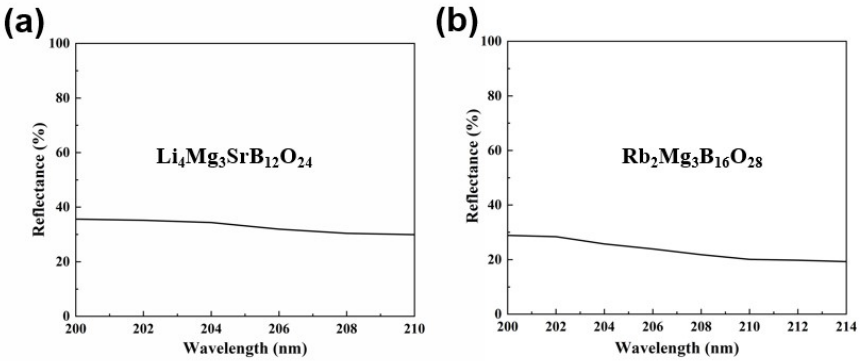

Figure S2. The UV-Vis-NIR diffuse reflectance spectroscopy curves in 200-210 nm of (a) $Li_4Mg_3SrB_{12}O_{24}$, and 200-214 nm of (b) $Rb_2Mg_3B_{16}O_{28}$.

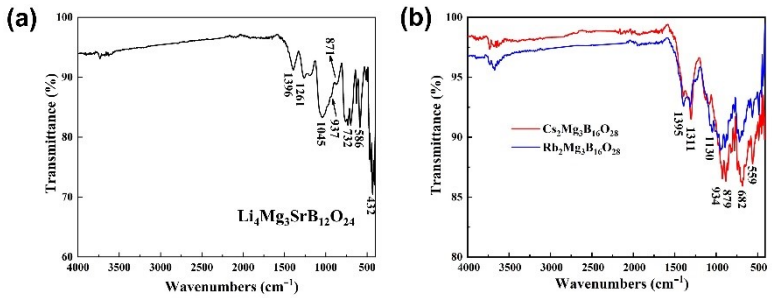

Figure S3. The IR spectra of (a) $Li_4Mg_3SrB_{12}O_{24}$, (b) $A_2Mg_3B_{16}O_{28}$ (A = Rb, Cs).

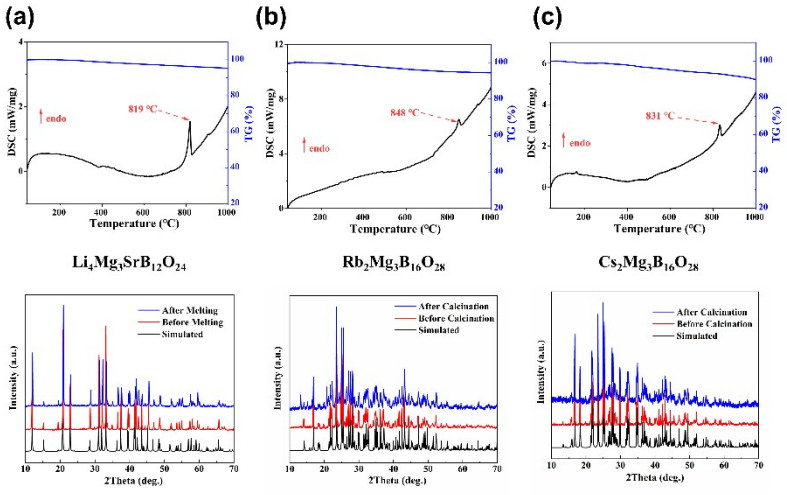

Figure S4. The TG-DSC curves and XRD patterns of the simulated, and before and after melting samples of (a) $Li_4Mg_3SrB_{12}O_{24}$, (b) $Rb_2Mg_3B_{16}O_{28}$, and (c) $Cs_2Mg_3B_{16}O_{28}$.