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Electronic Supporting Information

Synthesis, characterization and crystal structure of a new mixed alkali and alkaline-earth metal borate $Rb_9Ba_{24}(BO_3)_{19}$

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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) calculation for $Rb_9Ba_{24}(BO_3)_{19}$.

Atoms	*x*	*y*	*z*	*U*(eq)	BVS
Ba(1)	4375(1)	5625(1)	3539(1)	12(1)	1.8
Ba(2)	3032(1)	3032(1)	5000	9(1)	2.2
Ba(3)	0	3644(1)	0	10(1)	2.3
Ba(4)	1130(1)	2260(1)	1578(1)	16(1)	2.1
Rb(1)	0	0	5000	90(2)	0.9
Rb(2)	4668(1)	2334(1)	2062(2)	36(1)	0.8
Rb(3)	3333	6667	905(3)	39(1)	0.7
B(1)	2216(4)	4433(7)	2833(14)	10(2)	2.9
B(2)	5443(4)	4557(4)	2189(14)	10(2)	2.8
B(3)	2532(7)	1266(4)	2757(15)	13(2)	2.9
B(4)	0	0	0	40(1)	/
O(1)	2633(3)	5266(5)	3643(11)	27(2)	1.9
O(2)	2703(3)	3999(3)	2405(6)	13(1)	2.0
O(3)	4647(3)	3952(3)	3118(6)	16(1)	2.0
O(4)	5604(3)	4396(3)	422(9)	22(2)	1.7
O(5)	2644(3)	2026(3)	1806(6)	15(1)	2.0
O(6)	2412(5)	1206(3)	4621(8)	20(2)	1.8
O(7)	712(17)	356(9)	1080(40)	106(10)	1.7

Note: The BVS for the B(4) atom which is coordinated with disordered O(7) atoms was not calculated.

Table S2. Selected bond lengths (Å) and angles (°) for $Rb_9Ba_{24}(BO_3)_{19}$.

$Rb_9Ba_{24}B_{19}O_{54}$			
Rb(1)-O(7)#1	3.040(3)	Ba(2)-O(6)#1	2.745(3)
Rb(1)-O(7)#2	3.040(3)	Ba(2)-O(3)	2.749(5)
Rb(1)-O(7)#3	3.040(3)	Ba(2)-O(3)#16	2.749(5)
Rb(1)-O(7)#4	3.040(3)	Ba(2)-O(5)	2.764(4)
Rb(1)-O(7)	3.040(3)	Ba(2)-O(5)#16	2.764(4
Rb(1)-O(7)#5	3.040(3)	Ba(3)-O(2)#13	2.636(4)
Rb(1)-O(6)#4	3.557(8)	Ba(3)-O(2)#18	2.636(4)
Rb(1)-O(6)#3	3.557(8)	Ba(3)-O(3)#18	2.727(4)
Rb(1)-O(6)#1	3.557(8)	Ba(3)-O(3)#13	2.727(4)
Rb(1)-O(6)#2	3.557(8)	Ba(3)-O(5)#13	2.738(5)
Rb(1)-O(6)	3.557(8)	Ba(3)-O(5)#18	2.738(5)
Rb(1)-O(6)#5	3.557(8)	Ba(3)-O(4)#11	2.923(5)
Rb(2)-O(3)	2.870(5)	Ba(3)-O(4)#13	2.923(5)
Rb(2)-O(3)#6	2.870(5)	Ba(4)-O(6)#1	2.777(6)
Rb(2)-O(5)#6	3.212(5)	Ba(4)-O(5)	2.795(5)
Rb(2)-O(5)	3.212(5)	Ba(4)-O(5)#18	2.796(5)
Rb(2)-O(1)#4	3.249(8)	Ba(4)-O(5)#9	2.796(4)
Rb(2)-O(4)	3.263(5)	Ba(4)-O(5)#13	2.796(4)
Rb(2)-O(4)#7	3.263(5)	Ba(4)-O(2)#18	2.886(4)
Rb(2)-O(2)#8	3.602(5)	Ba(4)-O(2)	2.886(4)
Rb(2)-O(2)#9	3.602(5)	Ba(4)-O(7)	2.964(6)
Rb(3)-O(1)#11	2.866(8)	Ba(4)-O(7)#3	2.964(6)
Rb(3)-O(1)	2.866(8)	Ba(4)-O(7)#13	2.990(3)
Rb(3)-O(1)#12	2.866(8)	B(1)-O(1)	1.360(13)
Rb(3)-O(4)#10	3.272(7)	B(1)-O(2)#18	1.389(7)
Rb(3)-O(4)#13	3.272(7)	B(1)-O(2)	1.389(7)
Rb(3)-O(4)#14	3.272(7)	B(2)-O(4)	1.371(12)
Ba(1)-O(1)#12	2.706(16)	B(2)-O(3)#17	1.396(7)
Ba(1)-O(1)	2.706(17)	B(2)-O(3)	1.396(7)
Ba(1)-O(3)#15	2.829(4)	B(3)-O(6)	1.369(12)
Ba(1)-O(3)#16	2.829(4)	B(3)-O(5)#6	1.391(7)
Ba(1)-O(4)#10	2.886(6)	B(3)-O(5)	1.391(7)
Ba(1)-O(2)#17	2.920(4)	B(4)-O(7)#20	1.310(3)
Ba(1)-O(2)	2.920(4)	B(4)-O(7)#8	1.310(3)
Ba(1)-O(3)#17	3.112(5)	B(4)-O(7)#3	1.310(3)
Ba(1)-O(3)	3.112(5)	B(4)-O(7)#2	1.310(3)
Ba(2)-O(2)#16	2.738(4)	B(4)-O(7)#13	1.310(3)
Ba(2)-O(2)	2.738(4)	B(4)-O(7)	1.310(3)
Ba(2)-O(6)	2.745(3)		
O(1)-B(1)-O(2)#18	120.7(4)	O(7)#20-B(4)-O(7)#2	92.2(18)
O(1)-B(1)-O(2)	120.7(4)	O(7)#8-B(4)-O(7)#2	92.2(18)
O(2)#18-B(1)-O(2)	118.5(8)	O(7)#3-B(4)-O(7)#2	87.8(18)

O(4)-B(2)-O(3)#17	121.6(4)	O(7)#20-B(4)-O(7)#13	87.8(18)
O(4)-B(2)-O(3)	121.6(4)	O(7)#8-B(4)-O(7)#13	87.8(18)
O(3)#17-B(2)-O(3)	116.8(8)	O(7)#3-B(4)-O(7)#13	92.2(18)
O(6)-B(3)-O(5)#6	120.6(4)	O(7)#2-B(4)-O(7)#13	180.0(2)
O(6)-B(3)-O(5)	120.6(4)	O(7)#20-B(4)-O(7)	180.0(3)
O(5)#6-B(3)-O(5)	118.4(8)	O(7)#8-B(4)-O(7)	92.2(18)
O(7)#20-B(4)-O(7)#8	87.8(18)	O(7)#3-B(4)-O(7)	87.8(18)
O(7)#20-B(4)-O(7)#3	92.2(18)	O(7)#2-B(4)-O(7)	87.8(18)
O(7)#8-B(4)-O(7)#3	180.0(3)	O(7)#13-B(4)-O(7)	92.2(18)

Symmetry transformations used to generate equivalent atoms:

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

#7 -y+1,x-y,z #8 y,-x+y,-z #9 y,x,-z #10 -x+1,-y+1,-z #11 -x+y,-x+1,z #12 -y+1,x-y+1,z

#13 x-y,x,-z #14 y,-x+y+1,-z #15 -x+1,-y+1,-z+1 #16 y,x,-z+1 #17 -y+1,-x+1,z #18 -x+y,y,z

#19 -x+y+1,-x+1,z #20 -x,-y,-z #21 x,y,z-1

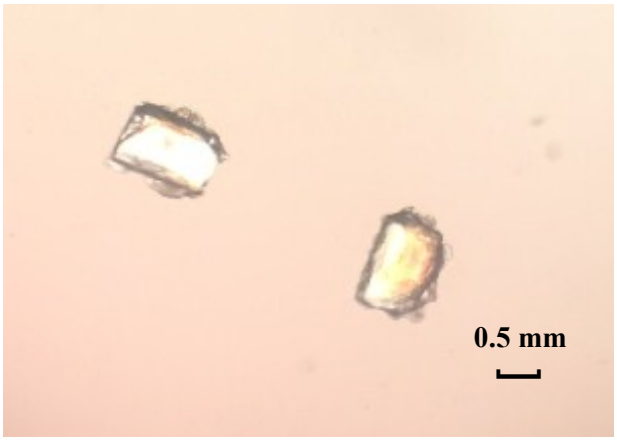

Figure S1: The crystal photo of $Rb_9Ba_{24}(BO_3)_{19}$.

Table S3. The Li^+/Rb^+ substitution in a series of anhydrous mixed alkali and alkaline-earth metal borates space group and B-O configurations in the structures.

Formula	Space group	FBB	Refs
$LiMgBO_3$	*C*2/*c*	Isolated BO_3 units	S1
$RbMgBO_3$	$P2_13$	Isolated BO_3 units	S2
$LiCaBO_3$	*Pbca*	Isolated BO_3 units	S3
$RbCaBO_3$	$P2_13$	Isolated BO_3units	S4
$Li_2Rb_7Sr_{24}(BO_3)_{19}$	$P\bar{3}m1$	Isolated BO_3 units	S5
$Rb_9Ba_{24}(BO_3)_{19}$	$P\bar{3}m1$	Isolated BO_3 units	This work

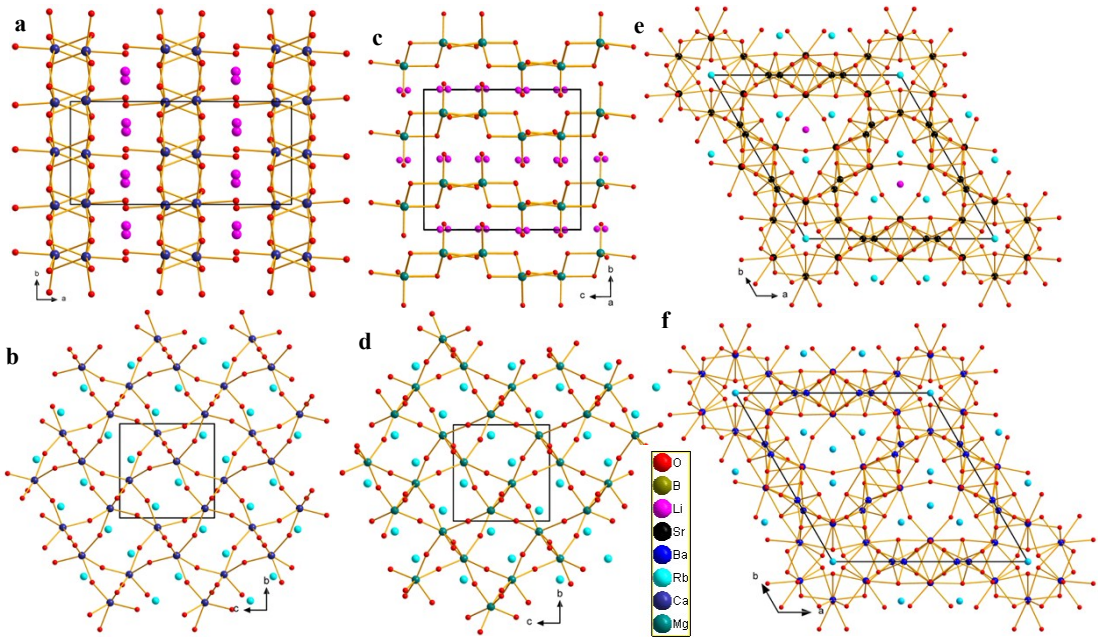

Figure S2. Crystal structures of (a) $LiCaBO_3$, (b) $RbCaBO_3$, (c) $LiMgBO_3$, (d) $RbMgBO_3$, (e) $Li_2Rb_7Sr_{24}(BO_3)_{19}$, (f) $Rb_9Ba_{24}(BO_3)_{19}$.

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