

Electronic Supplementary Information

**MBaYB₆O₁₂ (M = Rb, Cs): two new borates with large birefringence and short
ultraviolet cutoff edges**

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for RbBaYB₆O₁₂ (a) and CsBaYB₆O₁₂ (b). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atoms	Wyck.	x	y	z	$U(\text{eq})$
Rb(1)	c	0	0	-2170(20)	17(3)
Ba(1)	c	0	0	-2099(13)	16(1)
Y(1)	a	0	0	0	12(1)
B(1)	f	2827(8)	4500(8)	816(3)	18(1)
O(1)	f	2392(5)	2499(5)	798(2)	24(1)
O(2)	f	1229(5)	5052(5)	822(2)	25(1)

Atoms	Wyck.	x	y	z	$U(\text{eq})$
Cs(1)	c	0	0	7860(2)	39(2)
Ba(1)	c	0	0	7872(2)	8(1)
Y(1)	a	0	0	10000	13(1)
B(1)	f	1703(7)	4507(7)	10799(3)	26(1)
O(1)	f	3840(4)	5090(4)	10815(2)	33(1)
O(2)	f	182(5)	2525(4)	10791(2)	37(1)

Table S2. Selected bond lengths ($\text{\AA}$) and angles ($^\circ$) for RbBaYB₆O₁₂ (a) and CsBaYB₆O₁₂ (b).

(a) RbBaYB ₆ O ₁₂			
Rb(1)-O(1)#8	2.912(9)	O(1)#10-Rb(1)-O(1)#4	138.3(10)
Rb(1)-O(1)#9	2.912(9)	O(2)#11-Rb(1)-O(1)#4	67.9(3)
Rb(1)-O(1)#10	2.912(9)	O(2)#12-Rb(1)-O(1)#4	127.2(8)
Rb(1)-O(2)#11	2.949(8)	O(2)#13-Rb(1)-O(1)#4	105.6(5)
Rb(1)-O(2)#12	2.949(8)	O(1)#8-Rb(1)-O(1)#5	138.3(10)
Rb(1)-O(2)#13	2.949(8)	O(1)#9-Rb(1)-O(1)#5	88.2(4)

Rb(1)-O(1)#4	3.01(3)	O(1)#10-Rb(1)-O(1)#5	79.8(4)
Rb(1)-O(1)#5	3.01(3)	O(2)#11-Rb(1)-O(1)#5	127.2(8)
Rb(1)-O(1)#1	3.01(3)	O(2)#12-Rb(1)-O(1)#5	105.6(5)
Ba(1)-O(1)#4	2.909(18)	O(2)#13-Rb(1)-O(1)#5	67.9(3)
Ba(1)-O(1)#5	2.909(18)	O(1)#4-Rb(1)-O(1)#5	61.2(6)
Ba(1)-O(1)#1	2.909(18)	O(1)#8-Rb(1)-O(1)#1	79.8(4)
Ba(1)-O(1)#8	2.943(7)	O(1)#9-Rb(1)-O(1)#1	138.3(10)
Ba(1)-O(1)#9	2.943(7)	O(1)#10-Rb(1)-O(1)#1	88.2(4)
Ba(1)-O(1)#10	2.943(7)	O(2)#11-Rb(1)-O(1)#1	105.6(5)
Ba(1)-O(2)#11	2.978(7)	O(2)#12-Rb(1)-O(1)#1	67.9(3)
Ba(1)-O(2)#12	2.978(7)	O(2)#13-Rb(1)-O(1)#1	127.2(8)
Ba(1)-O(2)#13	2.978(7)	O(1)#4-Rb(1)-O(1)#1	61.2(6)
Y(1)-O(1)	2.268(3)	O(1)#5-Rb(1)-O(1)#1	61.2(6)
Y(1)-O(1)#1	2.268(3)	O(1)#4-Ba(1)-O(1)#5	63.6(5)
Y(1)-O(1)#2	2.268(3)	O(1)#4-Ba(1)-O(1)#1	63.6(5)
Y(1)-O(1)#3	2.268(3)	O(1)#5-Ba(1)-O(1)#1	63.6(5)
Y(1)-O(1)#4	2.268(3)	O(1)#4-Ba(1)-O(1)#8	89.6(3)
Y(1)-O(1)#5	2.268(3)	O(1)#5-Ba(1)-O(1)#8	142.1(7)
B(1)-O(1)	1.319(6)	O(1)#1-Ba(1)-O(1)#8	81.0(2)
B(1)-O(2)	1.399(6)	O(1)#4-Ba(1)-O(1)#9	81.0(2)
B(1)-O(2)#14	1.402(6)	O(1)#5-Ba(1)-O(1)#9	89.6(3)
O(1)-Y(1)-O(1)#1	180.00(14)	O(1)#1-Ba(1)-O(1)#9	142.1(7)
O(1)-Y(1)-O(1)#2	85.07(13)	O(1)#8-Ba(1)-O(1)#9	113.3(4)
O(1)#1-Y(1)-O(1)#2	94.93(14)	O(1)#4-Ba(1)-O(1)#10	142.1(7)
O(1)-Y(1)-O(1)#3	85.07(14)	O(1)#5-Ba(1)-O(1)#10	81.0(2)
O(1)#1-Y(1)-O(1)#3	94.93(14)	O(1)#1-Ba(1)-O(1)#10	89.6(3)
O(1)#2-Y(1)-O(1)#3	85.07(14)	O(1)#8-Ba(1)-O(1)#10	113.3(4)
O(1)-Y(1)-O(1)#4	94.93(13)	O(1)#9-Ba(1)-O(1)#10	113.3(4)

O(1)#1-Y(1)-O(1)#4	85.07(14)	O(1)#4-Ba(1)-O(2)#11	68.89(19)
O(1)#2-Y(1)-O(1)#4	180.00(14)	O(1)#5-Ba(1)-O(2)#11	130.2(5)
O(1)#3-Y(1)-O(1)#4	94.93(14)	O(1)#1-Ba(1)-O(2)#11	107.5(3)
O(1)-Y(1)-O(1)#5	94.93(13)	O(1)#8-Ba(1)-O(2)#11	47.02(13)
O(1)#1-Y(1)-O(1)#5	85.07(14)	O(1)#9-Ba(1)-O(2)#11	68.61(18)
O(1)#2-Y(1)-O(1)#5	94.93(14)	O(1)#10-Ba(1)-O(2)#11	148.5(8)
O(1)#3-Y(1)-O(1)#5	180.00(14)	O(1)#4-Ba(1)-O(2)#12	130.2(5)
O(1)#4-Y(1)-O(1)#5	85.07(14)	O(1)#5-Ba(1)-O(2)#12	107.5(3)
O(1)#8-Rb(1)-O(1)#9	115.2(5)	O(1)#1-Ba(1)-O(2)#12	68.89(19)
O(1)#8-Rb(1)-O(1)#10	115.2(5)	O(1)#8-Ba(1)-O(2)#12	68.61(18)
O(1)#9-Rb(1)-O(1)#10	115.2(5)	O(1)#9-Ba(1)-O(2)#12	148.5(8)
O(1)#8-Rb(1)-O(2)#11	47.53(16)	O(1)#10-Ba(1)-O(2)#12	47.02(13)
O(1)#9-Rb(1)-O(2)#11	69.4(2)	O(2)#11-Ba(1)-O(2)#12	114.2(3)
O(1)#10-Rb(1)-O(2)#11	152.9(12)	O(1)#4-Ba(1)-O(2)#13	107.5(3)
O(1)#8-Rb(1)-O(2)#12	69.4(2)	O(1)#5-Ba(1)-O(2)#13	68.89(19)
O(1)#9-Rb(1)-O(2)#12	152.9(12)	O(1)#1-Ba(1)-O(2)#13	130.2(5)
O(1)#10-Rb(1)-O(2)#12	47.52(16)	O(1)#8-Ba(1)-O(2)#13	148.5(8)
O(2)#11-Rb(1)-O(2)#12	115.9(4)	O(1)#9-Ba(1)-O(2)#13	47.02(13)
O(1)#8-Rb(1)-O(2)#13	152.9(12)	O(1)#10-Ba(1)-O(2)#13	68.61(18)
O(1)#9-Rb(1)-O(2)#13	47.52(16)	O(2)#11-Ba(1)-O(2)#13	114.2(3)
O(1)#10-Rb(1)-O(2)#13	69.4(2)	O(2)#12-Ba(1)-O(2)#13	114.2(3)
O(2)#11-Rb(1)-O(2)#13	115.9(4)	O(1)-B(1)-O(2)	122.4(4)
O(2)#12-Rb(1)-O(2)#13	115.9(4)	O(1)-B(1)-O(2)#14	120.5(4)
O(1)#8-Rb(1)-O(1)#4	88.2(4)	O(2)-B(1)-O(2)#14	117.1(4)
O(1)#9-Rb(1)-O(1)#4	79.8(4)		

Symmetry transformations used to generate equivalent atoms:

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

#7 $-x-2/3, -y-1/3, -z-1/3$	#8 $x-2/3, y-1/3, z-1/3$	#9 $-x+y+1/3, -x+2/3, z-1/3$
#10 $-y+1/3, x-y-1/3, z-1/3$	#11 $-y+1/3, x-y+2/3, z-1/3$	#12 $-x+y-2/3, -x-1/3, z-1/3$
#13 $x+1/3, y-1/3, z-1/3$	#14 $-y+1, x-y+1, z$	#15 $-x+1/3, -y+2/3, -z-1/3$
#16 $-x+y, -x+1, z$	#17 $x-1/3, y+1/3, z+1/3$	

(b) CsBaYB₆O₁₂

Cs(1)-O(2)#1	2.991(3)	O(1)#5-Cs(1)-O(2)#9	127.93(13)
Cs(1)-O(2)#2	2.991(3)	O(1)#6-Cs(1)-O(2)#9	107.30(11)
Cs(1)-O(2)#3	2.991(3)	O(2)#7-Cs(1)-O(2)#9	61.37(12)
Cs(1)-O(1)#4	2.998(3)	O(2)#8-Cs(1)-O(2)#9	61.37(12)
Cs(1)-O(1)#5	2.998(3)	O(2)#1-Ba(1)-O(2)#2	113.98(7)
Cs(1)-O(1)#6	2.998(3)	O(2)#1-Ba(1)-O(2)#3	113.98(7)
Cs(1)-O(2)#7	3.017(5)	O(2)#2-Ba(1)-O(2)#3	113.98(7)
Cs(1)-O(2)#8	3.017(5)	O(2)#1-Ba(1)-O(2)#7	81.98(10)
Cs(1)-O(2)#9	3.017(5)	O(2)#2-Ba(1)-O(2)#7	140.48(10)
Ba(1)-O(2)#1	2.996(3)	O(2)#3-Ba(1)-O(2)#7	88.38(11)
Ba(1)-O(2)#2	2.996(3)	O(2)#1-Ba(1)-O(2)#8	140.48(10)
Ba(1)-O(2)#3	2.996(3)	O(2)#2-Ba(1)-O(2)#8	88.38(11)
Ba(1)-O(2)#7	3.000(4)	O(2)#3-Ba(1)-O(2)#8	81.98(10)
Ba(1)-O(2)#8	3.000(4)	O(2)#7-Ba(1)-O(2)#8	61.76(10)
Ba(1)-O(2)#9	3.000(4)	O(2)#1-Ba(1)-O(2)#9	88.38(11)
Ba(1)-O(1)#4	3.003(3)	O(2)#2-Ba(1)-O(2)#9	81.98(10)
Ba(1)-O(1)#5	3.003(3)	O(2)#3-Ba(1)-O(2)#9	140.48(10)
Ba(1)-O(1)#6	3.003(3)	O(2)#7-Ba(1)-O(2)#9	61.76(10)
Y(1)-O(2)#8	2.281(3)	O(2)#8-Ba(1)-O(2)#9	61.76(10)
Y(1)-O(2)	2.281(3)	O(2)#1-Ba(1)-O(1)#4	46.30(8)
Y(1)-O(2)#10	2.281(3)	O(2)#2-Ba(1)-O(1)#4	69.73(8)
Y(1)-O(2)#9	2.281(3)	O(2)#3-Ba(1)-O(1)#4	149.48(12)
Y(1)-O(2)#7	2.281(3)	O(2)#7-Ba(1)-O(1)#4	107.62(9)

Y(1)-O(2)#11	2.281(3)	O(2)#8-Ba(1)-O(1)#4	128.41(10)
B(1)-O(2)	1.309(5)	O(2)#9-Ba(1)-O(1)#4	69.09(8)
B(1)-O(1)	1.394(5)	O(2)#1-Ba(1)-O(1)#5	69.73(8)
B(1)-O(1)#14	1.400(5)	O(2)#2-Ba(1)-O(1)#5	149.48(12)
O(2)#1-Cs(1)-O(2)#2	114.29(8)	O(2)#3-Ba(1)-O(1)#5	46.30(8)
O(2)#1-Cs(1)-O(2)#3	114.29(8)	O(2)#7-Ba(1)-O(1)#5	69.09(8)
O(2)#2-Cs(1)-O(2)#3	114.29(8)	O(2)#8-Ba(1)-O(1)#5	107.62(9)
O(2)#1-Cs(1)-O(1)#4	46.39(8)	O(2)#9-Ba(1)-O(1)#5	128.41(10)
O(2)#2-Cs(1)-O(1)#4	69.87(8)	O(1)#4-Ba(1)-O(1)#5	114.67(6)
O(2)#3-Cs(1)-O(1)#4	150.20(17)	O(2)#1-Ba(1)-O(1)#6	149.48(12)
O(2)#1-Cs(1)-O(1)#5	69.87(8)	O(2)#2-Ba(1)-O(1)#6	46.30(8)
O(2)#2-Cs(1)-O(1)#5	150.20(17)	O(2)#3-Ba(1)-O(1)#6	69.73(8)
O(2)#3-Cs(1)-O(1)#5	46.39(8)	O(2)#7-Ba(1)-O(1)#6	128.41(10)
O(1)#4-Cs(1)-O(1)#5	114.97(8)	O(2)#8-Ba(1)-O(1)#6	69.09(8)
O(2)#1-Cs(1)-O(1)#6	150.20(17)	O(2)#9-Ba(1)-O(1)#6	107.62(9)
O(2)#2-Cs(1)-O(1)#6	46.39(8)	O(1)#4-Ba(1)-O(1)#6	114.67(6)
O(2)#3-Cs(1)-O(1)#6	69.87(8)	O(1)#5-Ba(1)-O(1)#6	114.67(6)
O(1)#4-Cs(1)-O(1)#6	114.97(8)	O(2)#8-Y(1)-O(2)	180.000(2)
O(1)#5-Cs(1)-O(1)#6	114.96(8)	O(2)#8-Y(1)-O(2)#10	95.11(13)
O(2)#1-Cs(1)-O(2)#7	81.78(10)	O(2)-Y(1)-O(2)#10	84.89(13)
O(2)#2-Cs(1)-O(2)#7	139.85(14)	O(2)#8-Y(1)-O(2)#9	84.89(13)
O(2)#3-Cs(1)-O(2)#7	88.15(12)	O(2)-Y(1)-O(2)#9	95.11(13)
O(1)#4-Cs(1)-O(2)#7	107.30(11)	O(2)#10-Y(1)-O(2)#9	180.000(1)
O(1)#5-Cs(1)-O(2)#7	68.93(9)	O(2)#8-Y(1)-O(2)#7	84.89(13)
O(1)#6-Cs(1)-O(2)#7	127.93(13)	O(2)-Y(1)-O(2)#7	95.11(13)
O(2)#1-Cs(1)-O(2)#8	139.85(14)	O(2)#10-Y(1)-O(2)#7	95.11(13)
O(2)#2-Cs(1)-O(2)#8	88.15(12)	O(2)#9-Y(1)-O(2)#7	84.89(13)
O(2)#3-Cs(1)-O(2)#8	81.78(10)	O(2)#8-Y(1)-O(2)#11	95.11(13)
O(1)#4-Cs(1)-O(2)#8	127.93(13)	O(2)-Y(1)-O(2)#11	84.89(13)

O(1)#5-Cs(1)-O(2)#8	107.30(11)	O(2)#10-Y(1)-O(2)#11	84.89(13)
O(1)#6-Cs(1)-O(2)#8	68.93(9)	O(2)#9-Y(1)-O(2)#11	95.11(13)
O(2)#7-Cs(1)-O(2)#8	61.37(12)	O(2)#7-Y(1)-O(2)#11	180.000(1)
O(2)#1-Cs(1)-O(2)#9	88.15(11)	O(2)-B(1)-O(1)	122.5(4)
O(2)#2-Cs(1)-O(2)#9	81.78(10)	O(2)-B(1)-O(1)#14	121.0(4)
O(2)#3-Cs(1)-O(2)#9	139.85(14)	O(1)-B(1)-O(1)#14	116.5(3)
O(1)#4-Cs(1)-O(2)#9	68.93(9)		

Symmetry transformations used to generate equivalent atoms:

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

Figure S1 (a) The unit cell and **(b)** asymmetric cell of $\text{RbBaYB}_6\text{O}_{12}$.

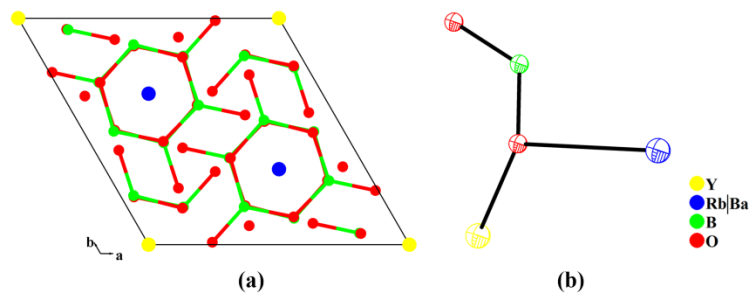
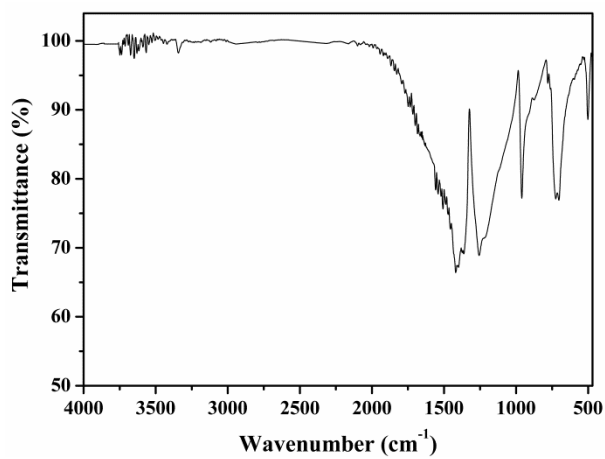
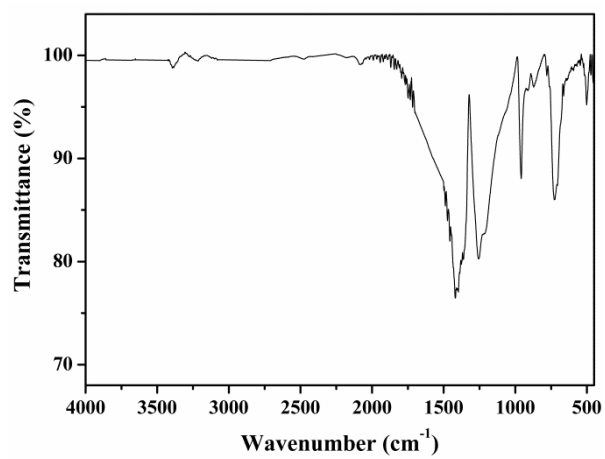


Figure S2 IR spectra of (a) $\text{RbBaYB}_6\text{O}_{12}$ and (b) $\text{CsBaYB}_6\text{O}_{12}$.



(a)



(b)

Figure S3 TG-DSC curves of **(a)** RbBaYB₆O₁₂ and **(b)** CsBaYB₆O₁₂.

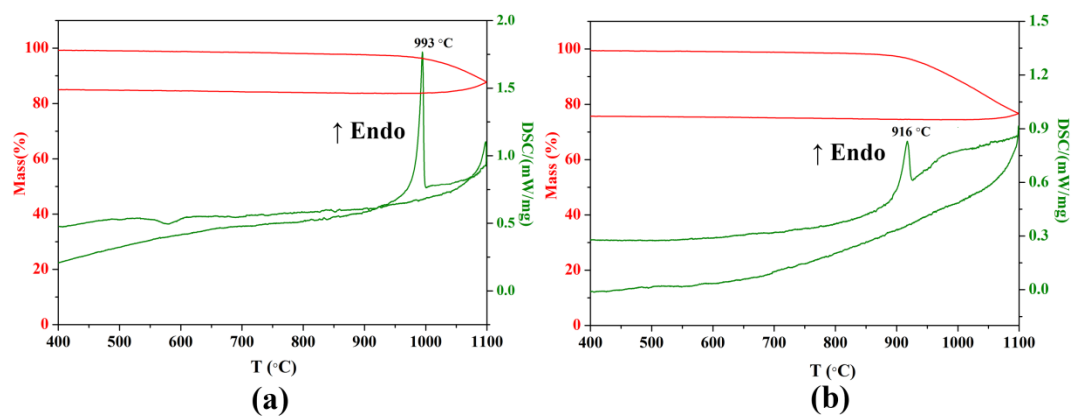


Figure S4 of **(a)** RbBaYB₆O₁₂ and **(b)** CsBaYB₆O₁₂.

