Supplementary Information (SI)

Synthesis, crystal structure and theoretical calculations of two rare-earth borates with DUV cut-off edges

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $YZnB_5O_{10}$. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x/a	y/b	z/c	U(e q)	BVS
Y(1)	8154(1)	6813(1)	7597(1)	6(1)	3.00
Zn(1)	8943(1)	5915(1)	3728(1)	7(1)	1.89
B(1)	5648(2)	6877(2)	888(2)	6(1)	2.92
B(2)	7772(2)	4680(2)	577(2)	6(1)	3.00
B(3)	5825(2)	4270(2)	2466(2)	6(1)	3.00
B(4)	4815(2)	1758(2)	3973(2)	5(1)	3.03
B(5)	6613(2)	3971(2)	5096(2)	6(1)	3.05
O(1)	4917(1)	8481(2)	709(1)	7(1)	1.81
O(2)	6808(1)	6253(2)	96(1)	7(1)	1.89
O(3)	8233(1)	3911(2)	-791(1)	6(1)	2.09
O(4)	6818(1)	3515(2)	1400(1)	6(1)	2.01
O(5)	5106(1)	5932(2)	1997(1)	7(1)	2.15
O(6)	4609(1)	2980(2)	2750(1)	6(1)	2.06
O(7)	6839(1)	4680(2)	3782(1)	7(1)	2.04
O(8)	5832(1)	300(2)	3493(1)	6(1)	1.87
O(9)	7459(1)	4423(2)	6293(1)	7(1)	1.87
O(10)	5476(1)	2677(2)	5236(1)	6(1)	2.09

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $GdZnB_5O_{10}$. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x/a	y/b	z/c	U(e q)	BVS
Gd(1)	4463(1)	6825(1)	2624(1)	5(1)	2.94
Zn(1)	9824(1)	5898(1)	8748(1)	7(1)	1.91
B(1)	7753(7)	4677(7)	5540(5)	5(1)	2.96
B(2)	5887(8)	6739(6)	6062(6)	4(1)	3.06
B(3)	10193(8)	6877(6)	5870(6)	5(1)	3.09
B(4)	11583(8)	4243(6)	7406(5)	5(1)	3.09
B(5)	6530(8)	8990(6)	4960(5)	5(1)	3.05
O(1)	7323(4)	5276(4)	6480(3)	5(1)	1.82
O(2)	9521(5)	3505(4)	6347(3)	5(1)	2.09
O(3)	5239(5)	7718(4)	4813(3)	4(1)	1.94
O(4)	6967(5)	7915(4)	7316(3)	5(1)	2.10
O(5)	11890(5)	4663(4)	8721(3)	6(1)	2.04
O(6)	10751(5)	8477(4)	5708(3)	6(1)	2.13
O(7)	6160(5)	9495(4)	3772(3)	7(1)	2.06
O(8)	5924(5)	3929(4)	4175(3)	5(1)	2.03
O(9)	8259(5)	6272(4)	5096(3)	7(1)	1.94
O(10)	11837(5)	5893(4)	6945(3)	6(1)	1.94

Table S3. Bond lengths [Å] and angles [deg] for YZnB$_5$O$_{10.}$

Y(1)-O(9)	2.2444(12)	B(1)-O(5)	1.366(2)
Y(1)-O(9)#1	2.3124(12)	B(1)-O(1)	1.373(2)
Y(1)-O(6)#2	2.3598(12)	B(2)-O(4)	1.455(2)
Y(1)-O(10)#1	2.3637(12)	B(2)-O(3)	1.482(2)
Y(1)-O(1)#3	2.4024(12)	B(2)-O(2)	1.501(2)
Y(1)-O(5)#3	2.4768(12)	B(2)-O(8)#4	1.502(2)
Y(1)-O(3)#4	2.5545(12)	B(3)-O(5)	1.458(2)
Y(1)-O(3)#5	2.6678(12)	B(3)-O(6)	1.462(2)
Y(1)-O(2)#5	2.7034(12)	B(3)-O(4)	1.466(2)
Y(1)-O(8)#6	2.8689(12)	B(3)-O(7)	1.490(2)
Zn(1)-O(7)	2.0265(12)	B(4)-O(10)	1.454(2)
Zn(1)-O(1)#3	2.0318(13)	B(4)-O(3)#8	1.471(2)
Zn(1)-O(4)#4	2.0794(12)	B(4)-O(6)	1.474(2)
Zn(1)-O(1)#7	2.1374(12)	B(4)-O(8)	1.493(2)
Zn(1)-O(8)#4	2.1503(12)	B(5)-O(9)	1.337(2)
Zn(1)-O(6)#4	2.4731(12)	B(5)-O(7)	1.366(2)
B(1)-O(2)	1.359(2)	B(5)-O(10)	1.391(2)
O(9)-Y(1)-O(9)#1	151.341(13)	O(3)#4-Y(1)-O(8)#6	150.04(4)
O(9)-Y(1)-O(6)#2	75.74(4)	O(3)#5-Y(1)-O(8)#6	51.91(3)
O(9)#1-Y(1)-O(6)#2	75.65(4)	O(2)#5-Y(1)-O(8)#6	91.92(3)
O(9)-Y(1)-O(10)#1	142.01(4)	O(7)-Zn(1)-O(1)#3	113.01(5)
O(9)#1-Y(1)-O(10)#1	59.39(4)	O(7)-Zn(1)-O(4)#4	99.66(5)
O(6)#2-Y(1)-O(10)#1	122.09(4)	O(1)#3-Zn(1)-O(4)#4	86.88(5)
O(9)-Y(1)-O(1)#3	71.39(4)	O(7)-Zn(1)-O(1)#7	88.97(5)
O(9)#1-Y(1)-O(1)#3	125.44(4)	O(1)#3-Zn(1)-O(1)#7	79.57(5)
O(6)#2-Y(1)-O(1)#3	124.81(4)	O(4)#4-Zn(1)-O(1)#7	165.99(5)
O(10)#1-Y(1)-O(1)#3	111.02(4)	O(7)-Zn(1)-O(8)#4	93.34(5)
O(9)-Y(1)-O(5)#3	126.38(4)	O(1)#3-Zn(1)-O(8)#4	150.81(5)
O(9)#1-Y(1)-O(5)#3	71.57(4)	O(4)#4-Zn(1)-O(8)#4	101.39(5)
O(6)#2-Y(1)-O(5)#3	126.94(4)	O(1)#7-Zn(1)-O(8)#4	89.00(5)
O(10)#1-Y(1)-O(5)#3	72.62(4)	O(7)-Zn(1)-O(6)#4	141.42(5)
O(1)#3-Y(1)-O(5)#3	55.69(4)	O(1)#3-Zn(1)-O(6)#4	100.23(4)
O(9)-Y(1)-O(3)#4	92.93(4)	O(4)#4-Zn(1)-O(6)#4	62.00(4)
O(9)#1-Y(1)-O(3)#4	69.75(4)	O(1)#7-Zn(1)-O(6)#4	116.80(4)
O(6)#2-Y(1)-O(3)#4	56.89(4)	O(8)#4-Zn(1)-O(6)#4	61.21(4)
O(10)#1-Y(1)-O(3)#4	125.06(4)	O(2)-B(1)-O(5)	121.62(15)
O(1)#3-Y(1)-O(3)#4	81.73(4)	O(2)-B(1)-O(1)	125.69(16)
O(5)#3-Y(1)-O(3)#4	72.96(4)	O(5)-B(1)-O(1)	112.68(15)
O(9)-Y(1)-O(3)#5	68.59(4)	O(4)-B(2)-O(3)	113.94(14)
O(9)#1-Y(1)-O(3)#5	116.90(4)	O(4)-B(2)-O(2)	109.19(13)
O(6)#2-Y(1)-O(3)#5	96.93(4)	O(3)-B(2)-O(2)	103.05(13)
O(10)#1-Y(1)-O(3)#5	75.67(4)	O(4)-B(2)-O(8)#4	109.38(14)

O(1)#3-Y(1)-O(3)#5	110.17(4)	O(3)-B(2)-O(8)#4	112.27(13)
O(5)#3-Y(1)-O(3)#5	134.97(4)	O(2)-B(2)-O(8)#4	108.71(13)
O(3)#4-Y(1)-O(3)#5	151.89(2)	O(5)-B(3)-O(6)	110.24(13)
O(9)-Y(1)-O(2)#5	103.34(4)	O(5)-B(3)-O(4)	112.54(14)
O(9)#1-Y(1)-O(2)#5	68.04(4)	O(6)-B(3)-O(4)	108.01(13)
O(6)#2-Y(1)-O(2)#5	69.75(4)	O(5)-B(3)-O(7)	106.09(13)
O(10)#1-Y(1)-O(2)#5	61.07(4)	O(6)-B(3)-O(7)	111.68(14)
O(1)#3-Y(1)-O(2)#5	160.36(4)	O(4)-B(3)-O(7)	108.31(13)
O(5)#3-Y(1)-O(2)#5	129.33(4)	O(10)-B(4)-O(3)#8	110.72(14)
O(3)#4-Y(1)-O(2)#5	117.76(4)	O(10)-B(4)-O(6)	110.40(13)
O(3)#5-Y(1)-O(2)#5	51.54(4)	O(3)#8-B(4)-O(6)	105.69(13)
O(9)-Y(1)-O(8)#6	83.28(4)	O(10)-B(4)-O(8)	113.48(13)
O(9)#1-Y(1)-O(8)#6	123.15(4)	O(3)#8-B(4)-O(8)	110.14(13)
O(6)#2-Y(1)-O(8)#6	147.59(4)	O(6)-B(4)-O(8)	106.02(13)
O(10)#1-Y(1)-O(8)#6	64.31(4)	O(9)-B(5)-O(7)	123.52(15)
O(1)#3-Y(1)-O(8)#6	68.86(4)	O(9)-B(5)-O(10)	116.25(15)
O(5)#3-Y(1)-O(8)#6	85.42(4)	O(7)-B(5)-O(10)	120.22(15)

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Bond lengths [Å] and angles [deg] for GdZnB$_5$O$_{10}$.

Gd(1)-O(1)	2.2778(17)	B(1)-O(5)	1.472(3)
Gd(1)-O(1)#1	2.3580(17)	B(1)-O(4)	1.474(3)
Gd(1)-O(2)#1	2.4175(17)	B(1)-O(3)	1.487(3)
Gd(1)-O(5)#2	2.4201(18)	B(2)-O(1)	1.336(3)
Gd(1)-O(10)#3	2.4512(18)	B(2)-O(6)	1.365(3)
Gd(1)-O(7)#3	2.5124(17)	B(2)-O(2)	1.392(3)
Gd(1)-O(4)#2	2.5782(17)	B(3)-O(7)	1.459(3)
Gd(1)-O(4)#4	2.6358(17)	B(3)-O(8)	1.463(3)
Gd(1)-O(9)#5	2.6742(18)	B(3)-O(5)	1.467(3)
Gd(1)-O(3)#4	2.8841(17)	B(3)-O(6)	1.495(3)
Zn(1)-O(6)	2.0304(17)	B(4)-O(8)	1.453(3)
Zn(1)-O(10)#3	2.0491(18)	B(4)-O(4)#8	1.483(3)
Zn(1)-O(8)#6	2.0813(18)	B(4)-O(3)#6	1.496(3)
Zn(1)-O(10)#7	2.1147(18)	B(4)-O(9)	1.501(3)
Zn(1)-O(3)#6	2.1962(17)	B(5)-O(9)	1.359(3)
Zn(1)-O(5)#6	2.4216(18)	B(5)-O(7)	1.369(3)
B(1)-O(2)	1.456(3)	B(5)-O(10)	1.374(3)
O(1)-Gd(1)-O(1)#1	150.685(19)	O(4)#2-Gd(1)-O(3)#4	150.42(5)
O(1)-Gd(1)-O(2)#1	145.14(6)	O(4)#4-Gd(1)-O(3)#4	51.85(5)
O(1)#1-Gd(1)-O(2)#1	58.32(6)	O(9)#5-Gd(1)-O(3)#4	91.87(5)
O(1)-Gd(1)-O(5)#2	74.96(6)	O(6)-Zn(1)-O(10)#3	116.87(7)
O(1)#1-Gd(1)-O(5)#2	76.03(6)	O(6)-Zn(1)-O(8)#6	99.50(7)
O(2)#1-Gd(1)-O(5)#2	121.64(6)	O(10)#3-Zn(1)-O(8)#6	86.52(7)
O(1)-Gd(1)-O(10)#3	71.09(6)	O(6)-Zn(1)-O(10)#7	89.52(7)
O(1)#1-Gd(1)-O(10)#3	124.89(6)	O(10)#3-Zn(1)-O(10)#7	79.28(8)
O(2)#1-Gd(1)-O(10)#3	110.23(6)	O(8)#6-Zn(1)-O(10)#7	165.53(7)
O(5)#2-Gd(1)-O(10)#3	125.83(6)	O(6)-Zn(1)-O(3)#6	91.27(7)
O(1)-Gd(1)-O(7)#3	124.37(6)	O(10)#3-Zn(1)-O(3)#6	149.06(7)
O(1)#1-Gd(1)-O(7)#3	71.19(6)	O(8)#6-Zn(1)-O(3)#6	102.04(7)
O(2)#1-Gd(1)-O(7)#3	73.50(6)	O(10)#7-Zn(1)-O(3)#6	88.95(7)
O(5)#2-Gd(1)-O(7)#3	125.74(6)	O(6)-Zn(1)-O(5)#6	139.93(7)
O(10)#3-Gd(1)-O(7)#3	54.88(6)	O(10)#3-Zn(1)-O(5)#6	98.55(7)
O(1)-Gd(1)-O(4)#2	89.69(6)	O(8)#6-Zn(1)-O(5)#6	62.76(7)
O(1)#1-Gd(1)-O(4)#2	70.56(6)	O(10)#7-Zn(1)-O(5)#6	116.37(7)
O(2)#1-Gd(1)-O(4)#2	125.16(5)	O(3)#6-Zn(1)-O(5)#6	61.27(6)
O(5)#2-Gd(1)-O(4)#2	56.15(6)	O(2)-B(1)-O(5)	110.55(19)
O(10)#3-Gd(1)-O(4)#2	82.57(6)	O(2)-B(1)-O(4)	110.1(2)
O(7)#3-Gd(1)-O(4)#2	72.51(5)	O(5)-B(1)-O(4)	106.2(2)
O(1)-Gd(1)-O(4)#4	70.66(6)	O(2)-B(1)-O(3)	114.0(2)
O(1)#1-Gd(1)-O(4)#4	117.62(6)	O(5)-B(1)-O(3)	105.8(2)
O(2)#1-Gd(1)-O(4)#4	76.52(6)	O(4)-B(1)-O(3)	109.83(19)
O(5)#2-Gd(1)-O(4)#4	97.54(5)	O(1)-B(2)-O(6)	122.9(2)

O(10)#3-Gd(1)-O(4)#4	109.06(6)	O(1)-B(2)-O(2)	117.1(2)
O(7)#3-Gd(1)-O(4)#4	135.82(5)	O(6)-B(2)-O(2)	120.0(2)
O(4)#2-Gd(1)-O(4)#4	151.30(3)	O(7)-B(3)-O(8)	112.6(2)
O(1)-Gd(1)-O(9)#5	104.63(6)	O(7)-B(3)-O(5)	110.7(2)
O(1)#1-Gd(1)-O(9)#5	68.45(6)	O(8)-B(3)-O(5)	107.5(2)
O(2)#1-Gd(1)-O(9)#5	61.57(6)	O(7)-B(3)-O(6)	105.93(19)
O(5)#2-Gd(1)-O(9)#5	69.40(6)	O(8)-B(3)-O(6)	108.4(2)
O(10)#3-Gd(1)-O(9)#5	159.84(6)	O(5)-B(3)-O(6)	111.7(2)
O(7)#3-Gd(1)-O(9)#5	130.58(5)	O(8)-B(4)-O(4)#8	113.7(2)
O(4)#2-Gd(1)-O(9)#5	117.43(5)	O(8)-B(4)-O(3)#6	109.6(2)
O(4)#4-Gd(1)-O(9)#5	52.23(5)	O(4)#8-B(4)-O(3)#6	112.6(2)
O(1)-Gd(1)-O(3)#4	86.37(6)	O(8)-B(4)-O(9)	109.1(2)
O(1)#1-Gd(1)-O(3)#4	121.49(5)	O(4)#8-B(4)-O(9)	103.11(19)
O(2)#1-Gd(1)-O(3)#4	63.79(5)	O(3)#6-B(4)-O(9)	108.49(19)
O(5)#2-Gd(1)-O(3)#4	148.56(5)	O(9)-B(5)-O(7)	121.3(2)
O(10)#3-Gd(1)-O(3)#4	68.42(5)	O(9)-B(5)-O(10)	125.6(2)
O(7)#3-Gd(1)-O(3)#4	85.67(5)	O(7)-B(5)-O(10)	113.1(2)

Symmetry transformations used to generate equivalent atoms:

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

Fig. S1. The picture is under a microscope of (a) $YZnB_5O_{10}$, (b) $GdZnB_5O_{10.}$
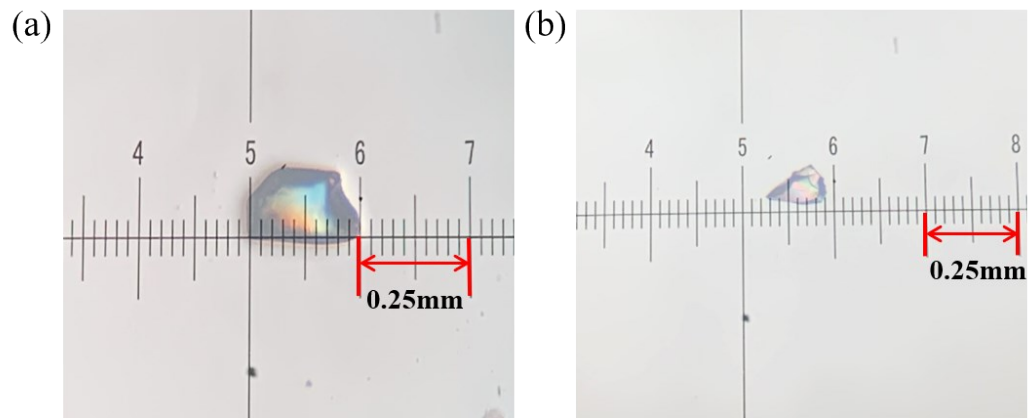
(a)

0.25mm

(b)

0.25mm

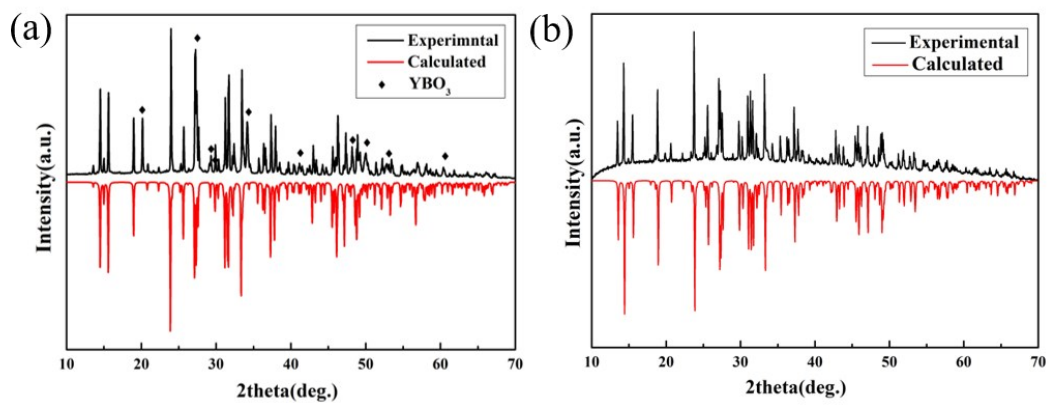**Fig. S2.** Calculated and experimental XRD patterns of (a) YZnB$_5$O$_{10}$, (b) GdZnB$_5$O$_{10}$.

Fig. S3. (a) Cation coordination environment of Zn in the $YZnB_5O_{10}$, (b) Cation coordination environment of Y in the $YZnB_5O_{10}$.