

Na₃YB₈O₁₅: a new rare-earth borate with an infinite one-dimensional

[B₈O₁₅]_∞ chain and short ultraviolet cutoff edge

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#The authors declare no competing financial interest.

Table S1. Crystal data and structure refinement for Na₃YB₈O₁₅.

Empirical formula	Na ₃ YB ₈ O ₁₅
Formula weight	484.36
Crystal system	Triclinic
Space group	<i>P</i> $\bar{1}$
<i>a</i> / Å	6.4122(2)
<i>b</i> / Å	7.3634(3)
<i>c</i> / Å	13.1781(5)
α / °	89.126(2)
β / °	78.657(2)
γ / °	66.8170(10)
Z, pcalcd / g·cm ⁻³	2, 2.875
Volume / Å ³	559.46(4)
Theta range for data collection	1.580 to 27.517
Reflections collected / unique	17964 / 2545 [<i>R</i> (int) = 0.0547]
Completeness (%)	98.6
Goodness-of-fit on <i>F</i> ²	1.147
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)] ^[a]	<i>R</i> ₁ = 0.0204, <i>wR</i> ₂ = 0.0607
<i>R</i> indices (all data) ^[a]	<i>R</i> ₁ = 0.0217, <i>wR</i> ₂ = 0.0612
Largest diff. peak and hole (e·Å ⁻³)	0.381 and -0.329

^[a]*R*₁ = Σ||*F*_o - |*F*_c||/Σ|*F*_o| and *wR*₂ = [Σ*w*(*F*_o² - *F*_c²)² / Σ*w* *F*_o⁴]^{1/2} for *F*_o² > 2σ(*F*_o²)

Table S2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Na}_3\text{YB}_8\text{O}_{15}$. U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atoms	x	y	z	U_{eq}
Na(1)	10380(2)	2696(2)	8884(1)	19(1)
Na(2)	7672(2)	2392(2)	4770(1)	20(1)
Na(3)	6244(2)	10952(2)	7647(1)	21(1)
Y(1)	-1008(1)	12512(1)	11708(1)	8(1)
B(1)	6524(5)	6129(4)	10149(2)	11(1)
B(2)	3282(5)	9207(4)	9933(2)	10(1)
B(3)	5943(4)	6991(4)	8353(2)	10(1)
B(4)	9010(4)	6411(4)	6677(2)	9(1)
B(5)	6314(5)	4805(4)	6842(2)	9(1)
B(6)	7815(5)	7851(4)	4969(2)	11(1)
B(7)	6803(4)	6295(4)	3608(2)	9(1)
B(8)	8433(5)	8872(4)	3216(2)	11(1)
O(1)	7874(3)	5031(3)	10758(1)	15(1)
O(2)	6959(3)	5628(2)	9098(1)	13(1)
O(3)	4596(3)	7889(3)	10563(1)	13(1)
O(4)	1511(3)	10855(3)	10335(1)	15(1)
O(5)	3865(3)	8715(2)	8868(1)	11(1)
O(6)	7728(3)	7513(2)	7701(1)	11(1)
O(7)	4944(3)	6110(3)	7663(1)	12(1)
O(8)	8468(3)	4725(2)	6469(1)	10(1)
O(9)	5569(3)	3538(2)	6429(1)	10(1)
O(10)	8507(3)	7847(2)	5877(1)	12(1)
O(11)	8304(3)	9170(2)	4283(1)	12(1)
O(12)	6709(3)	6755(2)	4710(1)	11(1)
O(13)	9548(3)	9699(3)	2523(1)	13(1)
O(14)	7329(3)	7738(2)	2930(1)	10(1)
O(15)	8502(3)	4258(2)	3280(1)	9(1)

Table S3. Bond distances [\AA] and angles [$^\circ$] for $\text{Na}_3\text{YB}_8\text{O}_{15}$.

Na(1)-O(1)	2.834(2)	O(11)#5-Na(2)-O(10)#3	97.34(7)
Na(1)-O(1)#2	2.446(2)	O(11)#5-Na(2)-O(11)#3	88.99(6)
Na(1)-O(2)	2.3661(19)	O(11)#5-Na(2)-O(12)#4	89.66(7)
Na(1)-O(4)#1	2.391(2)	O(11)#5-Na(2)-O(15)	112.83(7)
Na(1)-O(5)#1	2.9006(19)	O(12)#4-Na(2)-O(11)#3	137.96(6)
Na(1)-O(13)#3	2.559(2)	O(15)-Na(2)-O(11)#3	108.79(6)
Na(1)-O(14)#3	2.4988(19)	O(15)-Na(2)-O(12)#4	110.35(7)
Na(2)-O(9)	2.3046(19)	O(3)#6-Na(3)-O(5)	72.37(6)
Na(2)-O(10)#3	2.367(2)	O(3)#6-Na(3)-O(9)#7	114.86(7)
Na(2)-O(11)#3	2.903(2)	O(3)#6-Na(3)-O(10)	153.54(7)
Na(2)-O(11)#5	2.3224(19)	O(3)#6-Na(3)-O(13)#9	91.21(7)
Na(2)-O(12)#4	2.573(2)	O(5)-Na(3)-O(10)	93.98(5)
Na(2)-O(15)	2.4719(19)	O(6)-Na(3)-O(3)#6	103.45(7)
Na(3)-O(3)#6	2.405(2)	O(6)-Na(3)-O(5)	54.63(6)
Na(3)-O(5)	2.926(2)	O(6)-Na(3)-O(9)#7	141.52(8)
Na(3)-O(6)	2.3338(19)	O(6)-Na(3)-O(10)	51.34(6)
Na(3)-O(9)#7	2.434(2)	O(6)-Na(3)-O(13)#9	81.17(7)
Na(3)-O(10)	2.998(2)	O(6)-Na(3)-O(14)#8	113.03(7)
Na(3)-O(13)#9	2.512(2)	O(9)#7-Na(3)-O(5)	140.44(7)
Na(3)-O(14)#8	2.383(2)	O(9)#7-Na(3)-O(10)	90.24(6)
Y(1)-O(1)#11	2.1812(17)	O(9)#7-Na(3)-O(13)#9	94.17(7)
Y(1)-O(4)	2.1768(17)	O(13)#9-Na(3)-O(5)	125.19(6)
Y(1)-O(5)#10	2.5730(17)	O(13)#9-Na(3)-O(10)	78.09(6)
Y(1)-O(6)#6	2.3751(17)	O(14)#8-Na(3)-O(3)#6	106.92(7)
Y(1)-O(7)#10	2.2965(17)	O(14)#8-Na(3)-O(5)	80.63(6)
Y(1)-O(13)#12	2.2520(17)	O(14)#8-Na(3)-O(9)#7	59.87(6)
Y(1)-O(15)#13	2.3553(16)	O(14)#8-Na(3)-O(10)	92.54(6)
B(1)-O(1)	1.323(3)	O(14)#8-Na(3)-O(13)#9	152.65(8)
B(1)-O(2)	1.383(3)	O(1)#11-Y(1)-O(5)#10	89.38(6)
B(1)-O(3)	1.414(3)	O(1)#11-Y(1)-O(6)#6	107.76(6)
B(2)-O(3)	1.395(3)	O(1)#11-Y(1)-O(7)#10	78.09(7)
B(2)-O(4)	1.319(3)	O(1)#11-Y(1)-O(13)#12	166.00(7)
B(2)-O(5)	1.394(3)	O(1)#11-Y(1)-O(15)#13	98.45(6)
B(3)-O(2)	1.451(3)	O(4)-Y(1)-O(1)#11	87.62(7)
B(3)-O(5)	1.479(3)	O(4)-Y(1)-O(5)#10	87.19(6)
B(3)-O(6)	1.464(3)	O(4)-Y(1)-O(6)#6	84.75(6)
B(3)-O(7)	1.493(3)	O(4)-Y(1)-O(7)#10	140.16(6)
B(4)-O(6)	1.492(3)	O(4)-Y(1)-O(13)#12	90.90(7)
B(4)-O(8)	1.458(3)	O(4)-Y(1)-O(15)#13	144.24(6)
B(4)-O(10)	1.472(3)	O(6)#6-Y(1)-O(5)#10	160.68(6)
B(4)-O(15)#3	1.486(3)	O(7)#10-Y(1)-O(5)#10	56.06(5)
B(5)-O(7)	1.364(3)	O(7)#10-Y(1)-O(6)#6	134.98(6)
B(5)-O(8)	1.350(3)	O(7)#10-Y(1)-O(15)#13	75.22(6)
B(5)-O(9)	1.365(3)	O(13)#12-Y(1)-O(5)#10	76.63(6)
B(6)-O(10)	1.355(3)	O(13)#12-Y(1)-O(6)#6	85.94(6)
B(6)-O(11)	1.401(3)	O(13)#12-Y(1)-O(7)#10	94.38(6)
B(6)-O(12)	1.351(3)	O(13)#12-Y(1)-O(15)#13	90.88(6)

B(7)-O(9)#4	1.487(3)	O(15)#13-Y(1)-O(5)#10	127.83(5)
B(7)-O(12)	1.481(3)	O(15)#13-Y(1)-O(6)#6	59.77(6)
B(7)-O(14)	1.475(3)	O(1)-B(1)-O(2)	121.8(2)
B(7)-O(15)	1.473(3)	O(1)-B(1)-O(3)	120.1(2)
B(8)-O(11)	1.407(3)	O(2)-B(1)-O(3)	118.1(2)
B(8)-O(13)	1.336(3)	O(4)-B(2)-O(3)	121.1(2)
B(8)-O(14)	1.387(3)	O(4)-B(2)-O(5)	120.8(2)
O(1)#2-Na(1)-O(1)	69.62(7)	O(5)-B(2)-O(3)	118.1(2)
O(1)-Na(1)-O(5)#1	121.80(6)	O(2)-B(3)-O(5)	111.44(19)
O(1)#2-Na(1)-O(5)#1	106.81(7)	O(2)-B(3)-O(6)	109.4(2)
O(1)#2-Na(1)-O(13)#3	142.78(7)	O(2)-B(3)-O(7)	111.89(19)
O(1)#2-Na(1)-O(14)#3	86.66(7)	O(5)-B(3)-O(7)	101.47(18)
O(2)-Na(1)-O(1)#2	83.28(7)	O(6)-B(3)-O(5)	114.1(2)
O(2)-Na(1)-O(1)	53.18(6)	O(6)-B(3)-O(7)	108.26(19)
O(2)-Na(1)-O(4)#1	121.04(7)	O(8)-B(4)-O(6)	113.82(19)
O(2)-Na(1)-O(5)#1	166.93(7)	O(8)-B(4)-O(10)	111.74(19)
O(2)-Na(1)-O(13)#3	110.67(7)	O(8)-B(4)-O(15)#3	110.53(18)
O(2)-Na(1)-O(14)#3	110.10(7)	O(10)-B(4)-O(6)	107.24(18)
O(4)#1-Na(1)-O(1)	69.94(6)	O(10)-B(4)-O(15)#3	108.49(19)
O(4)#1-Na(1)-O(1)#2	91.43(7)	O(15)#3-B(4)-O(6)	104.64(18)
O(4)#1-Na(1)-O(5)#1	51.89(5)	O(7)-B(5)-O(9)	120.9(2)
O(4)#1-Na(1)-O(13)#3	108.18(7)	O(8)-B(5)-O(7)	118.9(2)
O(4)#1-Na(1)-O(14)#3	128.21(7)	O(8)-B(5)-O(9)	120.2(2)
O(13)#3-Na(1)-O(1)	146.45(7)	O(10)-B(6)-O(11)	113.7(2)
O(13)#3-Na(1)-O(5)#1	66.37(6)	O(12)-B(6)-O(10)	125.9(2)
O(14)#3-Na(1)-O(1)	151.48(7)	O(12)-B(6)-O(11)	120.4(2)
O(14)#3-Na(1)-O(5)#1	79.33(6)	O(12)-B(7)-O(9)#4	105.13(18)
O(14)#3-Na(1)-O(13)#3	56.27(6)	O(14)-B(7)-O(9)#4	108.50(19)
O(9)-Na(2)-O(10)#3	125.24(7)	O(14)-B(7)-O(12)	111.87(18)
O(9)-Na(2)-O(11)#3	85.69(6)	O(15)-B(7)-O(9)#4	110.00(18)
O(9)-Na(2)-O(11)#5	115.46(7)	O(15)-B(7)-O(12)	109.85(19)
O(9)-Na(2)-O(12)#4	57.46(6)	O(15)-B(7)-O(14)	111.29(19)
O(9)-Na(2)-O(15)	129.64(7)	O(13)-B(8)-O(11)	120.2(2)
O(10)#3-Na(2)-O(11)#3	50.71(6)	O(13)-B(8)-O(14)	122.4(2)
O(10)#3-Na(2)-O(12)#4	169.29(8)	O(14)-B(8)-O(11)	117.4(2)
O(10)#3-Na(2)-O(15)	59.43(6)		

Symmetry transformations used to generate equivalent atoms:

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

Table S4 The compounds reported in the Na₂O-Y₂O₃-B₂O₃ ternary system.

Compound	Space group	Cationic coordination	FBB
Na ₃ Y(BO ₃) ₂	<i>P2₁/c</i>	NaO ₄ , NaO ₆ , NaO ₇ , YO ₇	BO ₃
Na ₂ Y ₂ O(BO ₃) ₂	<i>P2₁/c</i>	NaO ₆ , YO ₈	BO ₃
Na ₃ Y ₃ (BO ₃) ₄	<i>P6₃mc</i>	NaO ₇ , YO ₈	BO ₃

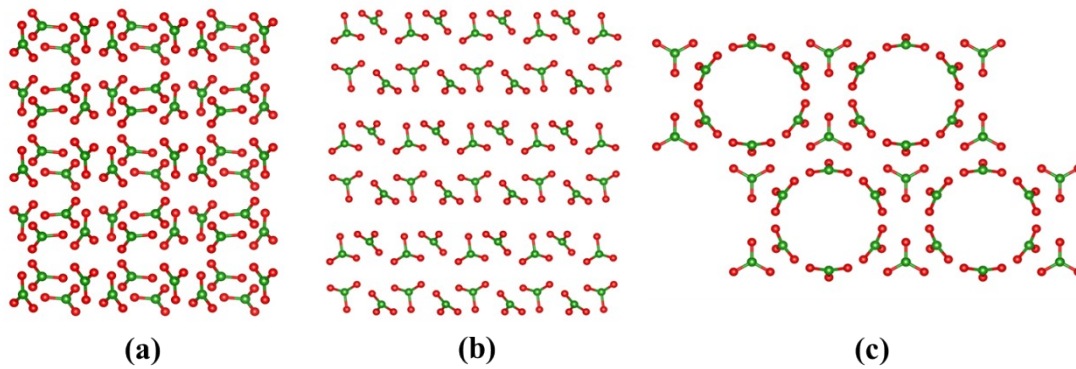


Figure S1 BO_3 anion frames in (a) $\text{Na}_3\text{Y}(\text{BO}_3)_2$, (b) $\text{Na}_2\text{Y}_2\text{O}(\text{BO}_3)_2$, and (c) $\text{Na}_3\text{Y}_3(\text{BO}_3)_4$.