Supporting Information

A new non-centrosymmetric Gd-based borate crystal $Rb_7SrGd_2(B_5O10)_3$: growth, structure, nonlinear optical and magnetic properties

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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) for $Rb_7SrGd_2(B_5O_{10})_3$.

U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)	BVS
Rb1	6667	3333	3333	22.1(5)	1.17
Rb2	4801(11)	0	0	27.9(4)	0.97
Rb3	3333	1274(12)	1667	21.8(3)	1.12
Sr1	6667	3333	-1667	7.6(4)	2.15
Gd1	6667	3333	628(5)	13.0(2)	2.87
B1	959(10)	-1352(10)	1305(7)	18(3)	3.03
B2	6667	758(12)	3333	17(3)	3.06
B3	7765(11)	1913(11)	-534(7)	17(3)	3.09
O1	7554(7)	2768(7)	-478(4)	21.5(17)	
O2	1014(7)	-634(7)	1931(4)	23.5(18)	
O3	4785(8)	-77(7)	2134(5)	36(3)	
O4	7690(7)	637(7)	3280(5)	22.7(16)	
O5	6631(6)	1382(6)	2558(5)	19.6(15)	

Table S2. Selected bond lengths for $Rb_7SrGd_2(B_5O_{10})_3$.

Atoms	Length/Å	Atoms	Length/Å
Rb1–O5[1]	2.867(8)	Rb3–O5[17]	2.849(8)
Rb1–O5[6]	2.867(8)	Rb3–O4[2]	3.011(8)
Rb1–O5[7]	2.867(8)	Rb3–O4[17]	3.011(8)
Rb1–O5[8]	2.867(8)	Sr1–O1	2.500(7)
Rb1–O5	2.867(8)	Gd1–O1	2.409(7)
Rb1–O5[2]	2.867(8)	Gd1–O1[1]	2.409(7)
Rb2–O3[14]	3.270(8)	Gd1–O1[2]	2.409(7)
Rb2–O3	3.270(8)	Gd1–O2[3]	2.276(7)
Rb2–O4[15]	2.942(8)	Gd1–O2[4]	2.276(7)
Rb2–O4[16]	2.942(8)	Gd1–O2[5]	2.276(7)
Rb2–O1[12]	3.147(8)	B1–O2	1.340(13)
Rb2–O1[2]	3.147(8)	B1[3]–O3	1.389(14)
Rb2–O2[13]	2.915(7)	B1[3]–O5	1.357(13)
Rb2–O2[3]	2.915(7)	B2–O5	1.471(12)
Rb3–O2	2.921(8)	B2–O4	1.472(12)
Rb3–O2[3]	2.921(8)	B3–O1	1.322(13)
Rb3–O3	3.354(10)	B3[15]–O4	1.377(14)
Rb3–O3[3]	3.354(10)	B3[18]–O3	1.411(12)
Rb3–O5[2]	2.849(8)		

[1]1-Y,+X-Y,+Z; [2]1+Y-X,1-X,+Z; [3]2/3-X,1/3-X+Y,1/3-Z; [4]2/3-Y+X,1/3-Y,1/3-Z; [5]2/3+Y,1/3+X,1/3-Z; [6]1/3-Y+X,2/3-Y,2/3-Z; [7]1/3+Y,-1/3+X,2/3-Z; [8]4/3-X,2/3-X+Y,2/3-Z; [9]2/3-Y,1/3+X-Y,1/3+Z; [10]2/3+X,1/3+Y,1/3+Z; [11]2/3+Y-X,1/3-X,1/3+Z; [12]+Y,-1+X,-Z; [13]1/3-Y,-1/3+X-Y,-1/3+Z; [14]-Y+X,-Y,-Z; [15]4/3+Y-X,2/3-X,-1/3+Z; [16]2/3+Y,-2/3+X,1/3-Z; [17]-1/3-Y+X,1/3-Y,1/3-Z; [18]2/3-Y,-2/3+X-Y,1/3+Z

Table S3 Selected bond angles for $Rb_7SrGd_2(B_5O_{10})_3$.

Atoms	Angle/°	Atoms	Angle/°
O1-Gd1-O1[1]	76.0(2)	O2[3]-Gd1-O2[4]	95.3(2)
O1-Gd1-O1[2]	76.0(2)	O2-B1-O3[5]	118.5(10)
O1[2]-Gd1-O1[1]	76.0(2)	O2-B1-O5[5]	122.4(10)
O2[4]-Gd1-O1[1]	86.5(2)	O5[5]-B1-O3[5]	119.0(9)
O2[4]-Gd1-O1	162.3(3)	O5-B2-O5[6]	107.8(12)
O2[3]-Gd1-O1	86.5(2)	O5[6]-B2-O4	111.3(4)
O2[4]-Gd1-O1[2]	102.0(3)	O5-B2-O4[6]	111.3(4)
O2[5]-Gd1-O1[1]	162.3(3)	O5-B2-O4	108.7(4)
O2[3]-Gd1-O1[1]	102.0(3)	O5[6]-B2-O4[6]	108.7(4)
O2[3]-Gd1-O1[2]	162.3(3)	O4-B2-O4[6]	109.1(12)
O2[5]-Gd1-O1	102.0(3)	O1- B3- O3[14]	121.1(10)
O2[5]-Gd1-O1[2]	86.5(3)	O1-B3-O4[16]	121.2(9)
O2[5]-Gd1-O2[4]	95.3(2)	O4[16]-B3-O3[14]	117.6(9)
O2[3]-Gd1-O2[5]	95.3(2)		

[1]1-Y, +X-Y, +Z; [2]1+Y-X, 1-X, +Z; [3]2/3-X, 1/3-X+Y, 1/3-Z; [4]2/3-Y+X, 1/3-Y, 1/3-Z; [5]2/3+Y, 1/3+X, 1/3-Z; [6]1/3-Y+X, 2/3-Y, 2/3-Z; [7]4/3-X, 2/3-X+Y, 2/3-Z; [8]1/3+Y, -1/3+X, 2/3-Z; [9]2/3+X, 1/3+Y, 1/3+Z; [10]2/3-Y, 1/3+X-Y, 1/3+Z; [11]2/3+Y-X, 1/3-X, 1/3+Z; [12]+Y, -1+X, -Z; [13]1/3-Y, -1/3+X-Y, -1/3+Z; [14]-Y+X, -Y, -Z; [15]2/3+Y, -2/3+X, 1/3-Z; [16]4/3+Y-X, 2/3-X, -1/3+Z; [17]-1/3-Y+X, 1/3-Y, 1/3-Z; [18]1+Y, +X, -Z; [19]2/3-Y, -2/3+X-Y, 1/3+Z; [20]1/3+Y-X, 2/3-X, -1/3+Z; [21]4/3-X, 2/3-X+Y, -1/3-Z; [22]1/3+Y, -1/3+X, -1/3-Z; [23]1/3-Y+X, 2/3-Y, -1/3-Z

Table S4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for $Rb_7SrGd_2(B_5O_{10})_3$.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd1	12.9(3)	12.9(3)	13.1(3)	0	0	6.43(14)
Rb1	14.0(6)	14.0(6)	38.4(12)	0	0	7.0(3)
Rb2	23.0(7)	25.2(8)	36.1(8)	-15.5(6)	-7.8(3)	12.6(4)
Rb3	14.0(7)	26.0(6)	21.6(7)	-0.8(2)	-1.6(5)	7.0(3)
O1	25(4)	24(4)	24(3)	0(3)	0(3)	19(4)
O2	31(5)	24(5)	21(3)	-7(3)	-2(3)	18(4)
O3	32(6)	21(4)	34(4)	9(3)	-23(4)	-2(4)
O5	19(4)	15(4)	23(4)	3(3)	-2(3)	6(3)
O4	26(4)	29(4)	24(4)	-13(3)	-8(3)	22(4)
B3	22(7)	26(7)	18(5)	-5(5)	0(5)	22(6)
B2	13(8)	17(6)	20(7)	-2(3)	-4(5)	7(4)
B1	21(7)	19(6)	19(5)	-2(4)	-2(4)	15(6)
Sr1	10.6(6)	10.6(6)	1.6(7)	0	0	5.3(3)

Table S5. Assignments of the infrared absorption peaks for $Rb_7SrGd_2(B_5O_{10})_3$.

Mode description	$Rb_7SrGd_2(B_5O_{10})_3$ (cm^{-1})
asymmetric stretching of $[BO_3]^{3-}$	1363, 1250, 1190
asymmetric stretching vibrations $[BO_4]^{5-}$	1034, 933
symmetric stretching of $[B_5O_{10}]^{5-}$	777, 734
bending vibrations of $[BO_3]^{3-}$ and $[BO_4]^{5-}$	487−611