Supporting Information

Two Scandium borate UV NLO crystals designed through chemical element substitution

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EXPERIMENTAL SECTION

Crystal Synthesis.

Polycrystalline RNSSBO specimens were synthesized via high-temperature solid-state reaction. Stoichiometric amounts of Sc_2O_3, Rb_2CO_3, Na_2CO_3, $SrCO_3$, and B_2O_3 were precisely weighed without additional purification. The reagents underwent thoroughly mixed in an agate mortar to ensure compositional uniformity, followed by transfer to an alumina crucible for pre-annealing at 400 °C for 24 hours within a muffle furnace. Subsequently, the mixture underwent sintering at temperatures exceeding 730 °C for 72 hours, with intermittent regrinding to optimize reaction completion, resulting in the desired crystalline sample. Single crystals of RNSSBO and NRSSBO were prepared via the high-temperature solution method, utilizing Na_2CO_3-B_2O_3 as a flux with spontaneous crystallization technique.

Single-Crystal Structure Determination.

To determine the structure of the title compound, single crystal with good quality was selected to characterize its structure. The crystallographic data of RNSSBO and NRSSBO crystals were recorded on a Bruker SMART APEX II 4K CCD diffractometer with Mo Kα radiation (λ = 0.71073 Å) at 298(2) K. The APEX3 software was applied to carry out the data integration and absorption corrections. The preliminary crystal structures were solved using SHELXT and refined with the SHELXL program within the Olex2 software package.[1-5] The structural symmetry was determined by using the PLATON program for eliminating symmetry elements to ensure the high degree of symmetry in the crystal structure.[6] Detailed crystallographic information and crystal structure refinements are presented in Tables S1.

Additionally, we applied the "EXYZ" and "EADP" constraints to accurately model the observed disorder. The relative occupancies were determined using a free "FAVR" command. For RNSSBO, the Sc and Sr sites were found to be disordered, and subsequently, disorder was also observed in two distinct Rb sites. The occupancies of each site were freely refined to $Rb(1)_{0.70}Na(1)_{0.30}$, $Rb(2)_{0.67}Na(2)_{0.33}$, $Sr(1)_{0.66}Sc(1)_{0.34,}$ and $Sc(2)_{0.84}Sr(2)_{0.16}$. For NRSSBO, the same disorder was observed, and the occupancies of each site were freely refined to $Rb(1)_{0.52}Na(1)_{0.48}$, $Na(2)_{0.53}Rb(2)_{0.47}$, $Sr(1)_{0.49}Sc(1)_{0.51,}$ and $Sc(2)_{0.85}Sr(2)_{0.15}$.

Powder X-ray diffraction.

The polycrystalline powder XRD test of the title compound was performed at room temperature by utilizing a Rigaku Smart-Lab 9kW X-ray diffractometer with Cu Kα radiation (λ =1.5418 Å). The scanning angle range (2θ) for the test was from 5 to 70°, with a scan step width 0.01° and a rate of 2s/step.

Thermal Analysis.

Thermal gravimetric (TG) and differential scanning calorimetry (DSC) analyses of RNSSBO were carried out using a HITACHI STA 200 TG/DSC thermal analyzer. The powder sample was placed in an alumina crucible and heated up to 1000 °C at a rate of 10 °C/min under a nitrogen atmosphere.

Elemental Analysis.

To evaluate the elemental distribution and atomic ratio in RNSSBO and NRSSBO compounds, small single-crystal samples stored in silicone oil were analyzed using an FEI Quanta FEG 250 field emission scanning electron microscope.

Optical Spectrum Measurements.

UV-vis-NIR diffuse reflectance spectra for RNSSBO were performed using a Lambda 750 UV-vis-NIR spectrophotometer with a wavelength range from 190 to 1200 nm at room temperature. The experimental bandgap of the title compound was determined based on the Kubelka−Munk function: $F(R) = (1-R)^2/2R = K/S$,[7]

where *R* represents reflectance, K represents absorption, and S represents scattering. Infrared spectra were analyzed using a Nicolet 50FT-IR spectrometer in the range of 500-2000 cm^{-1}.

Powder Second Harmonic Generation (SHG) Measurements.

Powder second-harmonic generation (SHG) measurements for RNSSBO were conducted via the Kurtz-Perry technique,[8] with wavelength of 1064 nm, pulse width of 10 ns and pulse repetition rate of 5 Hz, a Q-switched Nd: YAG laser was used to measure RNSSBO polycrystalline powders with different particle sizes. Commercial KH_2PO_4 (KDP) single crystals were identically fractionated as the benchmark reference.

Theoretical Calculation Details.

The computational analysis in this study was based on the crystallographic parameters obtained from RNSSBO and NRSSO crystals, respectively. Electronic structures and optical characteristics were modeled through density functional theory (DFT) utilizing the CASTEP computational suite.[9-12] The norm-conserving pseudopotential (NCP) framework[13] was employed to define the valence electrons for each element: Rb $5s^1$, Na $3s^1$, Sr $5s^2$, Sc $3d^14s^2$, B $2s^22p^1$, and O $2s^22p^4$. Exchange-correlation energies were treated with the Perdew-Burke-Ernzerhof (PBE) functional under the generalized gradient approximation (GGA) to ensure the accurate representation of electronic and structural properties. A kinetic energy cutoff of 800 eV was chosen for RNSSBO and NRSSBO. The numerical integration of the Brillouin zone was performed using 3 × 3 × 2 Monkhorst-Pack k-point sampling method.[14]

Table S1 Crystallographic data and structural refinement for $Rb_{4.1}Na_{2.9}SrSc_2(B_5O_{10})_3$ and $Na_4Rb_3Sr_{0.8}Sc_{2.2}(B_5O_{10})_3$

empirical formula	$Rb_{4.1}Na_{2.9}SrSc_2(B_5O_{10})_3$	$Na_4Rb_3Sr_{0.8}Sc_{2.2}(B_5O_{10})_3$
formula weight	1237.13	1158.26
temperature	297 K	297 K
crystal system	Trigonal	Trigonal
space group	*R*32	*R32*
a (Å)	12.9240(3)	12.8969 (13)
b (Å)	12.9240(3)	12.8969 (13)
c (Å)	15.1974(5)	14.891(2)
Z	3	3
V (Å^3)	2198.33(13)	2145.0(5)
Density (Mg/m^3)	2.803	2.690
R (int)	0.0498	0.1215
GOF (F^2)	1.056	1.037
Flack parameter	0.034 (12)	-0.01 (2)
final R indices [I>2σ (I)][a]	R_1=0.0358, wR_2=0.0706	R_1=0.0543, wR_2=0.0926
CCDC number	2496913	2496914

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$; $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

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Table S2. Atomic coordinates, equivalent isotropic displacement parameters and bond valence sum (BVS) for $Rb_{4.1}Na_{2.9}SrSc_2(B_5O_{10})_3$. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)	BVS
Na(3)	6667	3333	3333	42(2)	1.10
O(1)	5629(6)	5797(6)	3421(4)	56(2)	2.16
O(2)	4885(6)	4966(6)	2038(4)	58(2)	1.95
O(3)	6588(5)	4938(5)	2564(4)	49(2)	2.17
O(4)	4027(6)	5920(6)	2855(4)	58(2)	1.89
O(5)	5707(7)	3981(6)	1242(4)	57(2)	2.08
B(1)	4822(8)	5573(9)	2783(7)	41(2)	3.15
B(2)	6667	5661(11)	3333	46(3)	3.18
B(3)	5745(9)	4612(9)	1946(7)	41(2)	3.13
$Rb(1)_{0.70}Na(1)_{0.30}$	4585(1)	4585(1)	5000	41(1)	1.01
$Rb(2)_{0.67}Na(2)_{0.33}$	4873(1)	4873(1)	0	43(1)	1.08
$Sr(1)_{0.66}Sc(1)_{0.34}$	3333	6667	1667	26(1)	2.19
$Sc(2)_{0.84}Sr(2)_{0.16}$	6667	3333	553(1)	23(1)	3.02

Table S3. Atomic coordinates, equivalent isotropic displacement parameters and bond valence sum (BVS) for $Na_4Rb_3Sr_{0.8}Sc_{2.2}(B_5O_{10})_3$. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)	BVS
Na(3)	6667	3333	3333	46(3)	1.13
O(1)	5629(8)	5794(9)	3428(6)	62(3)	2.13
O(2)	4895(8)	4998(9)	2005(6)	64(3)	1.94
O(3)	6583(8)	4927(7)	2545(6)	54(3)	2.16
O(4)	5644(10)	3941(9)	1205(6)	68(3)	2.09
O(5)	4083(9)	5991(9)	2810(6)	62(3)	1.94
B(1)	4855(13)	5619(14)	2764(13)	50(5)	3.20
B(2)	6667	5650(16)	3333	46(6)	3.16
B(3)	5735(14)	4609(13)	1917(12)	46(4)	3.10
$Rb(1)_{0.52}Na(1)_{0.48}$	4602(2)	4602(2)	5000	47(1)	0.94
$Na(2)_{0.53}Rb(2)_{0.47}$	4857(3)	4857(3)	0	53(1)	0.83
$Sr(1)_{0.49}Sc(1)_{0.51}$	3333	6667	1667	26(1)	2.48
$Sc(2)_{0.85}Sr(2)_{0.15}$	6667	3333	564(2)	27(1)	2.99

Table S4. Bond lengths (Å) and angles (deg.) for $Rb_{4.1}Na_{2.9}SrSc_2(B_5O_{10})_3$

Na(3)-O(3)#1	2.427(6)	O(3)#1-Na(3)-O(3)#4	124.0(3)
Na(3)-O(3)#2	2.427(6)	O(3)#5-Na(3)-O(3)	124.0(3)
Na(3)-O(3)#3	2.427(6)	O(3)#5-Na(3)-O(3)#2	98.71(17)
Na(3)-O(3)#4	2.427(6)	O(3)#1-Na(3)-O(3)#5	98.72(17)
Na(3)-O(3)#5	2.427(6)	O(3)#1-Na(3)-O(3)#2	98.71(17)
Na(3)-O(3)	2.427(6)	O(3)#4-Na(3)-O(3)#5	132.1(3)
O(1)-B(2)	1.443(10)	O(3)#4-Na(3)-O(3)	98.71(17)
O(1)-B(1)	1.345(11)	O(3)#1-Na(3)-O(3)#3	132.1(3)
O(1)-Rb(2)#7	3.008(6)	O(3)#3-Na(3)-O(3)	98.71(17)
O(1)-Rb(1)	2.815(7)	O(3)#4-Na(3)-O(3)#3	98.71(17)
O(2)-B(1)	1.402(11)	O(3)#4-Na(3)-O(3)#2	57.8(3)
O(2)-B(3)	1.404(11)	O(3)#5-Na(3)-O(3)#3	57.8(3)
O(2)-Rb(2)	3.100(6)	O(3)#3-Na(3)-O(3)#2	124.0(3)
O(2)-Rb(1)#6	3.280(7)	O(3)#1-Na(3)-O(3)	57.8(3)
O(3)-B(2)	1.469(10)	O(3)-Na(3)-O(3)#2	132.1(3)
O(3)-B(3)	1.336(11)	O(1)#1-B(2)-O(1)	108.2(11)
O(3)-Rb(1)#8	2.900(6)	O(1)-B(2)-O(3)	112.2(3)
O(4)-B(1)	1.315(10)	O(1)#1-B(2)-O(3)#1	112.2(3)
O(4)-Rb(2)#7	3.427(8)	O(1)#1-B(2)-O(3)	109.1(4)
O(4)-Rb(2)#9	3.223(8)	O(1)-B(2)-O(3)#1	109.1(4)
O(4)-Sr(1)	2.421(6)	O(3)-B(2)-O(3)#1	106.0(10)
O(4)-Sc(2)#10	2.249(6)	O(1)-B(1)-O(2)	116.5(7)
O(5)-B(3)	1.331(11)	O(4)-B(1)-O(1)	121.4(9)
O(5)-Rb(2)	2.701(6)	O(4)-B(1)-O(2)	122.1(9)
O(5)-Rb(1)#6	2.885(7)	O(3)-B(3)-O(2)	118.7(8)
O(5)-Sc(2)	2.092(6)	O(5)-B(3)-O(2)	119.1(9)
		O(5)-B(3)-O(3)	122.1(8)
		O(1)#8-Rb(2)-O(1)#11	45.8(2)
		O(1)#8-Rb(2)-O(2)#12	90.72(17)

O(1)#8-Rb(2)-O(2)	86.97(17)	O(1)#14-Rb(1)-O(2)#5	122.79(17)
O(1)#11-Rb(2)-O(2)#12	86.97(17)	O(1)-Rb(1)-O(3)#7	93.27(16)
O(1)#11-Rb(2)-O(2)	90.72(17)	O(1)#14-Rb(1)-O(3)#7	49.05(17)
O(1)#8-Rb(2)-O(4)#6	90.58(15)	O(1)#14-Rb(1)-O(3)#1	93.26(16)
O(1)#11-Rb(2)-O(4)#13	90.58(15)	O(1)-Rb(1)-O(3)#1	49.05(17)
O(1)#11-Rb(2)-O(4)#6	133.19(15)	O(1)-Rb(1)-O(5)#9	85.00(16)
O(1)#8-Rb(2)-O(4)#13	133.19(15)	O(1)-Rb(1)-O(5)#5	114.70(17)
O(2)#12-Rb(2)-O(2)	177.5(3)	O(1)#14-Rb(1)-O(5)#9	114.70(17)
O(2)-Rb(2)-O(4)#6	105.07(16)	O(1)#14-Rb(1)-O(5)#5	85.00(16)
O(2)-Rb(2)-O(4)#13	75.91(16)	O(2)#5-Rb(1)-O(2)#9	67.68(19)
O(2)#12-Rb(2)-O(4)#6	75.91(16)	O(3)#7-Rb(1)-O(2)#5	156.09(15)
O(2)#12-Rb(2)-O(4)#13	105.07(16)	O(3)#1-Rb(1)-O(2)#9	156.09(15)
O(4)#6-Rb(2)-O(4)#13	135.71(18)	O(3)#7-Rb(1)-O(2)#9	92.61(15)
O(5)-Rb(2)-O(1)#11	108.66(19)	O(3)#1-Rb(1)-O(2)#5	92.61(15)
O(5)#12-Rb(2)-O(1)#8	108.66(19)	O(3)#7-Rb(1)-O(3)#1	109.4(2)
O(5)#12-Rb(2)-O(1)#11	72.89(19)	O(5)#9-Rb(1)-O(2)#9	44.41(16)
O(5)-Rb(2)-O(1)#8	72.89(19)	O(5)#5-Rb(1)-O(2)#9	100.60(17)
O(5)-Rb(2)-O(2)#12	132.67(16)	O(5)#5-Rb(1)-O(2)#5	44.41(16)
O(5)-Rb(2)-O(2)	47.37(16)	O(5)#9-Rb(1)-O(2)#5	100.60(17)
O(5)#12-Rb(2)-O(2)#12	47.37(16)	O(5)#9-Rb(1)-O(3)#7	71.04(17)
O(5)#12-Rb(2)-O(2)	132.67(16)	O(5)#5-Rb(1)-O(3)#7	133.93(16)
O(5)#12-Rb(2)-O(4)#6	118.65(18)	O(5)#5-Rb(1)-O(3)#1	71.04(17)
O(5)-Rb(2)-O(4)#13	118.65(18)	O(5)#9-Rb(1)-O(3)#1	133.93(16)
O(5)#12-Rb(2)-O(4)#13	60.66(17)	O(5)#9-Rb(1)-O(5)#5	142.8(2)
O(5)-Rb(2)-O(4)#6	60.66(17)	O(4)#15-Sr(1)-O(4)#13	70.5(2)
O(5)#12-Rb(2)-O(5)	178.4(3)	O(4)#15-Sr(1)-O(4)#16	108.6(3)
O(1)#14-Rb(1)-O(1)	117.6(3)	O(4)#15-Sr(1)-O(4)#11	70.5(2)
O(1)-Rb(1)-O(2)#5	108.60(15)	O(4)#17-Sr(1)-O(4)#16	70.4(2)
O(1)-Rb(1)-O(2)#9	122.79(17)	O(4)#11-Sr(1)-O(4)#16	178.4(4)
O(1)#14-Rb(1)-O(2)#9	108.60(15)	O(4)#16-Sr(1)-O(4)	70.5(2)

O(4)#15-Sr(1)-O(4)	178.4(4)	O(5)-Sc(2)-O(4)#6	88.3(3)
O(4)#13-Sr(1)-O(4)#11	70.5(2)	O(5)#3-Sc(2)-O(4)#6	96.5(2)
O(4)#11-Sr(1)-O(4)	110.6(3)	O(5)#3-Sc(2)-O(4)#18	88.3(3)
O(4)#13-Sr(1)-O(4)	108.6(3)	O(5)#4-Sc(2)-O(4)#8	88.3(3)
O(4)#15-Sr(1)-O(4)#17	110.6(3)	O(5)#4-Sc(2)-O(4)#18	96.5(2)
O(4)#17-Sr(1)-O(4)	70.5(2)	O(5)#3-Sc(2)-O(4)#8	164.6(2)
O(4)#13-Sr(1)-O(4)#17	178.4(4)	O(5)-Sc(2)-O(4)#18	164.6(2)
O(4)#11-Sr(1)-O(4)#17	108.6(3)	O(5)#4-Sc(2)-O(4)#6	164.6(3)
O(4)#13-Sr(1)-O(4)#16	110.6(3)	O(5)-Sc(2)-O(4)#8	96.5(2)
O(4)#18-Sc(2)-O(4)#6	76.8(2)	O(5)#4-Sc(2)-O(5)#3	97.1(2)
O(4)#18-Sc(2)-O(4)#8	76.8(2)	O(5)#3-Sc(2)-O(5)	97.1(2)
O(4)#6-Sc(2)-O(4)#8	76.8(2)	O(5)#4-Sc(2)-O(5)	97.1(2)

Symmetry transformations used to generate equivalent atoms:

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

Table S5. Bond lengths (Å) and angles (deg.) for $Na_4Rb_3Sr_{0.8}Sc_{2.2}(B_5O_{10})_3$

Na(3)-O(3)#1	2.416(8)	O(3)#1-Na(3)-O(3)#4	98.4(2)
Na(3)-O(3)#2	2.416(8)	O(3)#5-Na(3)-O(3)	98.4(2)
Na(3)-O(3)#3	2.416(8)	O(3)#5-Na(3)-O(3)#2	58.4(4)
Na(3)-O(3)#4	2.416(8)	O(3)#1-Na(3)-O(3)#5	123.9(4)
Na(3)-O(3)#5	2.416(8)	O(3)#1-Na(3)-O(3)#2	98.4(2)
Na(3)-O(3)	2.416(8)	O(3)#4-Na(3)-O(3)#5	132.4(4)
O(1)-B(1)	1.341(18)	O(3)#4-Na(3)-O(3)	123.9(4)
O(1)-B(2)	1.448(15)	O(3)#1-Na(3)-O(3)#3	132.4(4)
O(1)-Rb(2)#7	3.024(10)	O(3)#3-Na(3)-O(3)	98.4(2)
O(1)-Rb(1)	2.750(10)	O(3)#4-Na(3)-O(3)#3	58.4(4)
O(2)-B(1)	1.401(19)	O(3)#4-Na(3)-O(3)#2	98.4(2)
O(2)-B(3)	1.409(16)	O(3)#5-Na(3)-O(3)#3	98.4(2)
O(2)-Rb(2)	2.990(9)	O(3)#3-Na(3)-O(3)#2	123.9(4)
O(2)-Rb(1)#6	3.318(10)	O(3)#1-Na(3)-O(3)	58.4(4)
O(3)-B(2)	1.469(14)	O(3)-Na(3)-O(3)#2	132.4(4)
O(3)-B(3)	1.338(17)	O(1)-B(1)-O(2)	117.0(11)
O(3)-Rb(1)#8	2.863(9)	O(5)-B(1)-O(1)	122.7(15)
O(4)-B(3)	1.334(17)	O(5)-B(1)-O(2)	120.4(15)
O(4)-Rb(2)	2.617(9)	O(1)#1-B(2)-O(1)	107.5(15)
O(4)-Rb(1)#6	2.828(11)	O(1)#1-B(2)-O(3)#1	112.3(5)
O(4)-Sc(2)	2.073(9)	O(1)-B(2)-O(3)	112.3(5)
O(5)-B(1)	1.305(16)	O(1)#1-B(2)-O(3)	109.0(5)
O(5)-Rb(2)#9	3.302(11)	O(1)-B(2)-O(3)#1	109.0(5)
O(5)-Rb(2)#7	3.362(11)	O(3)-B(2)-O(3)#1	106.6(15)
O(5)-Sr(1)	2.331(8)	O(3)-B(3)-O(2)	118.8(13)
O(5)-Sc(2)#10	2.272(8)	O(4)-B(3)-O(2)	117.9(14)
		O(4)-B(3)-O(3)	123.2(13)
		O(1)#8-Rb(2)-O(1)#11	45.4(3)
		O(1)#11-Rb(2)-O(5)#6	132.4(2)

O(1)#11-Rb(2)-O(5)#12	90.4(2)	O(1)#14-Rb(1)-O(2)#9	110.0(2)
O(1)#8-Rb(2)-O(5)#6	90.4(2)	O(1)-Rb(1)-O(3)#1	50.0(2)
O(1)#8-Rb(2)-O(5)#12	132.4(2)	O(1)#14-Rb(1)-O(3)#7	50.0(2)
O(2)#13-Rb(2)-O(1)#8	89.8(2)	O(1)#14-Rb(1)-O(3)#1	92.5(3)
O(2)#13-Rb(2)-O(1)#11	86.1(3)	O(1)-Rb(1)-O(3)#7	92.5(3)
O(2)-Rb(2)-O(1)#8	86.1(3)	O(1)-Rb(1)-O(4)#4	116.1(3)
O(2)-Rb(2)-O(1)#11	89.8(2)	O(1)-Rb(1)-O(4)#9	84.4(2)
O(2)-Rb(2)-O(2)#13	175.6(4)	O(1)#14-Rb(1)-O(4)#9	116.1(3)
O(2)-Rb(2)-O(5)#6	106.5(2)	O(1)#14-Rb(1)-O(4)#4	84.4(2)
O(2)#13-Rb(2)-O(5)#12	106.5(2)	O(2)#4-Rb(1)-O(2)#9	66.4(3)
O(2)-Rb(2)-O(5)#12	75.2(2)	O(3)#7-Rb(1)-O(2)#4	155.2(2)
O(2)#13-Rb(2)-O(5)#6	75.2(2)	O(3)#7-Rb(1)-O(2)#9	93.2(2)
O(4)-Rb(2)-O(1)#11	109.9(3)	O(3)#1-Rb(1)-O(2)#9	155.2(2)
O(4)#13-Rb(2)-O(1)#11	73.7(3)	O(3)#1-Rb(1)-O(2)#4	93.2(2)
O(4)-Rb(2)-O(1)#8	73.7(3)	O(3)#7-Rb(1)-O(3)#1	109.7(4)
O(4)#13-Rb(2)-O(1)#8	109.9(3)	O(4)#9-Rb(1)-O(2)#9	44.1(2)
O(4)#13-Rb(2)-O(2)#13	49.0(2)	O(4)#9-Rb(1)-O(2)#4	99.7(2)
O(4)-Rb(2)-O(2)#13	131.2(2)	O(4)#4-Rb(1)-O(2)#9	99.7(2)
O(4)-Rb(2)-O(2)	49.0(2)	O(4)#4-Rb(1)-O(2)#4	44.1(2)
O(4)#13-Rb(2)-O(2)	131.2(2)	O(4)#4-Rb(1)-O(3)#7	134.2(2)
O(4)-Rb(2)-O(4)#13	176.4(5)	O(4)#9-Rb(1)-O(3)#1	134.2(2)
O(4)#13-Rb(2)-O(5)#6	118.7(3)	O(4)#4-Rb(1)-O(3)#1	71.4(2)
O(4)-Rb(2)-O(5)#12	118.7(3)	O(4)#9-Rb(1)-O(3)#7	71.4(2)
O(4)-Rb(2)-O(5)#6	59.8(2)	O(4)#9-Rb(1)-O(4)#4	141.6(4)
O(4)#13-Rb(2)-O(5)#12	59.8(2)	O(5)-Sr(1)-O(5)#15	72.6(3)
O(5)#6-Rb(2)-O(5)#12	136.7(3)	O(5)#16-Sr(1)-O(5)#12	72.6(3)
O(1)#14-Rb(1)-O(1)	117.3(4)	O(5)#16-Sr(1)-O(5)#11	72.6(3)
O(1)-Rb(1)-O(2)#9	122.0(3)	O(5)#12-Sr(1)-O(5)#17	106.0(5)
O(1)-Rb(1)-O(2)#4	110.0(2)	O(5)-Sr(1)-O(5)#17	72.6(3)
O(1)#14-Rb(1)-O(2)#4	122.0(3)	O(5)#12-Sr(1)-O(5)#11	72.6(3)

O(5)#16-Sr(1)-O(5)	177.6(6)	O(4)#3-Sc(2)-O(5)#6	94.7(4)
O(5)#16-Sr(1)-O(5)#17	108.9(5)	O(4)-Sc(2)-O(5)#8	94.7(4)
O(5)#12-Sr(1)-O(5)	108.9(5)	O(4)#3-Sc(2)-O(5)#18	87.5(4)
O(5)#11-Sr(1)-O(5)#17	177.6(5)	O(4)#5-Sc(2)-O(5)#8	87.5(4)
O(5)#16-Sr(1)-O(5)#15	106.0(4)	O(4)#5-Sc(2)-O(5)#6	161.2(4)
O(5)#15-Sr(1)-O(5)#17	72.6(3)	O(4)#5-Sc(2)-O(5)#18	94.7(4)
O(5)#12-Sr(1)-O(5)#15	177.6(6)	O(4)-Sc(2)-O(5)#6	87.5(4)
O(5)#11-Sr(1)-O(5)#15	108.9(5)	O(4)#3-Sc(2)-O(5)#8	161.2(4)
O(5)#11-Sr(1)-O(5)	106.0(5)	O(5)#18-Sc(2)-O(5)#8	74.8(3)
O(4)-Sc(2)-O(4)#3	100.5(3)	O(5)#6-Sc(2)-O(5)#8	74.8(3)
O(4)#5-Sc(2)-O(4)	100.5(3)	O(5)#18-Sc(2)-O(5)#6	74.8(3)
O(4)#5-Sc(2)-O(4)#3	100.5(3)	O(4)-Sc(2)-O(5)#18	161.2(4)

Symmetry transformations used to generate equivalent atoms:

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

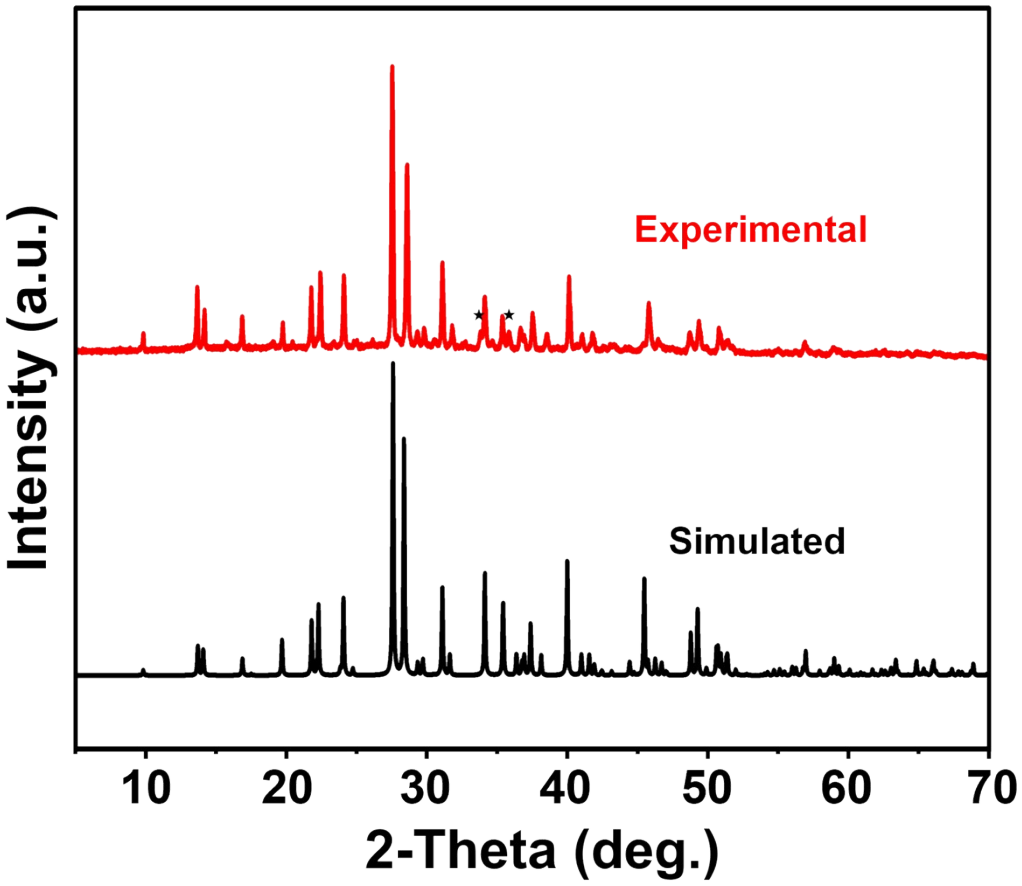

Figure S1. Experimental and calculated PXRD patterns of RNSSBO. (Two faint impurity peak observed near 35 degree attributed to the $NaScB_2O_5$ and $RbNa_2BO_3$ phase.)

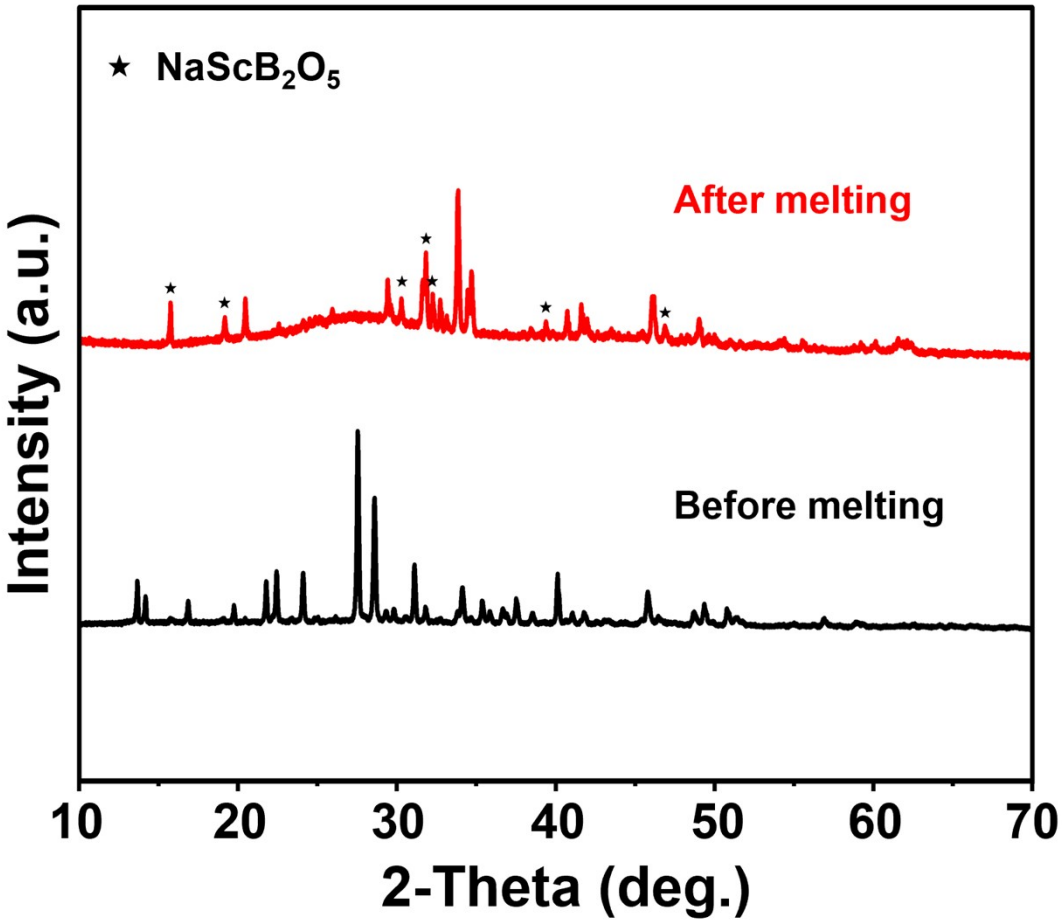

Figure S2 Experimental PXRD patterns of RNSSBO after and before melting process.

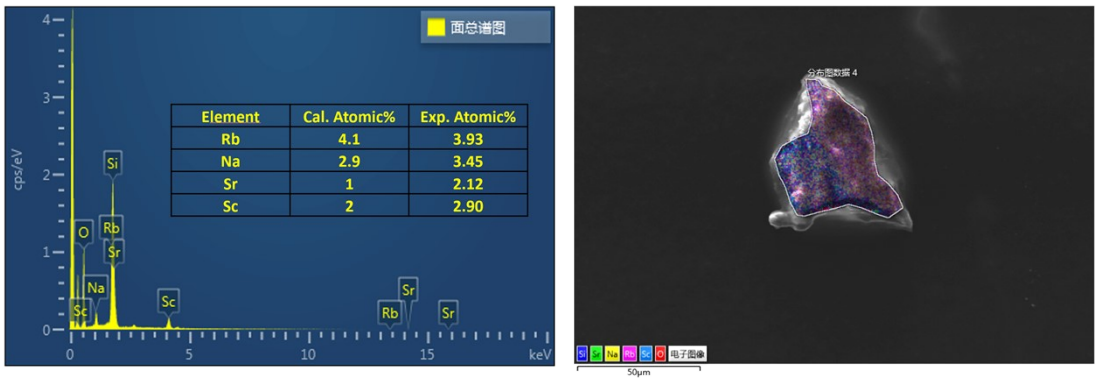

Figure S3. The EDS spectra of RNSSBO crystal. (The observed silicon peak originates from the silicone oil used for sample preservation.)

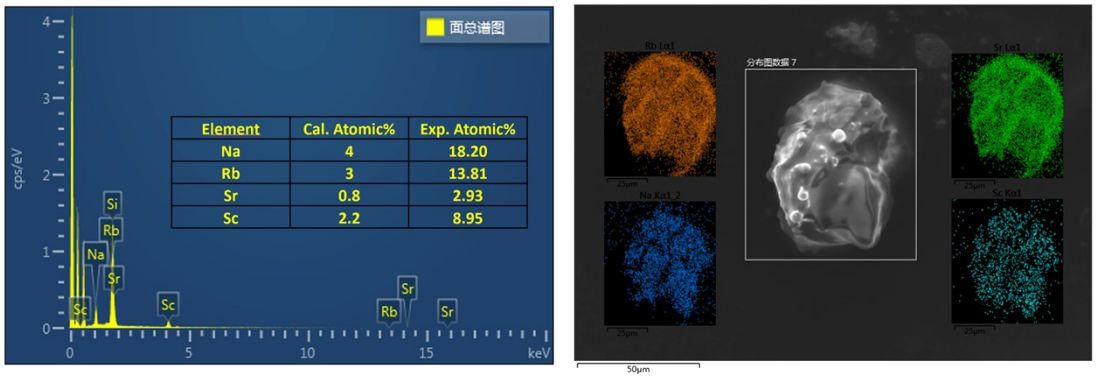

Figure S4. The EDS spectra of NRSSBO crystal. (The observed silicon peak originates from the silicone oil used for sample preservation.)

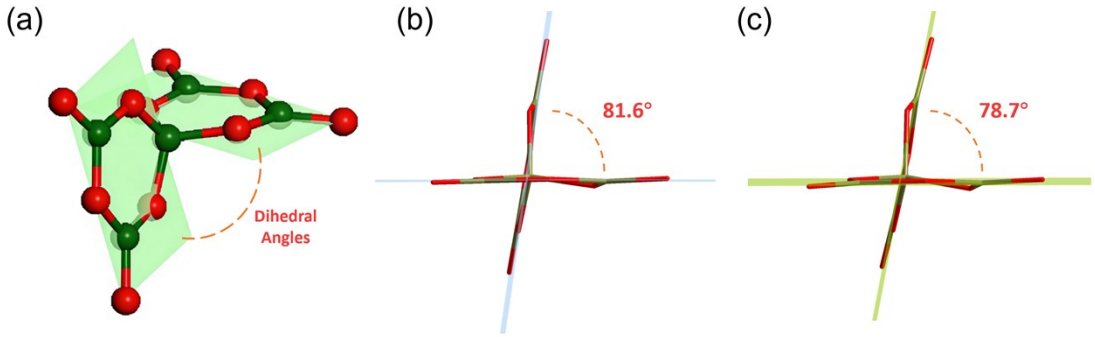

Figure S5. The dihedral angles of (a) $[B_5O_{10}]$ groups in (b) RNSSBO and (c) NRSSBO, respectively.

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