Electronic Supplementary information for

Two Non-Centrosymmetric Mixed Alkali Metal and Alkaline Earth Metal Scandium Borate Nonlinear Optical Materials with Short Ultraviolet Cutoff Edges

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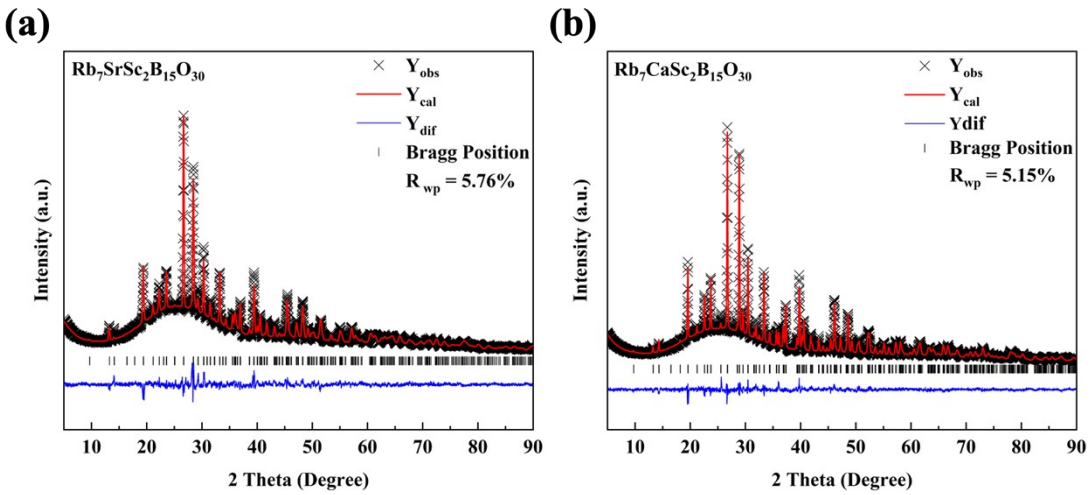

Figure S1. Refined powder XRD patterns of (a) $Rb_7SrSc_2B_{15}O_{30}$ and (b) $Rb_7CaSc_2B_{15}O_{30}$: the red line and blue line show calculated data and the difference, respectively; the black "×" and black "|" are the experimental data and Bragg positions of samples, respectively.

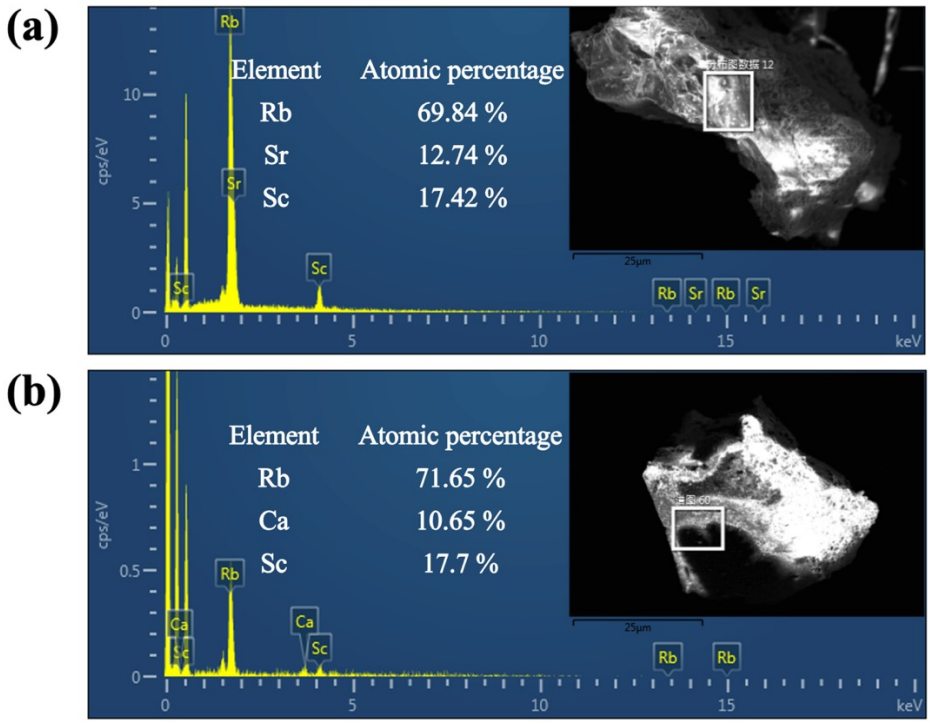

Figure S2. The heavy element analysis spectra and atomic percentages of (a) $Rb_7SrSc_2B_{15}O_{30}$ and (b) $Rb_7CaSc_2B_{15}O_{30}$.

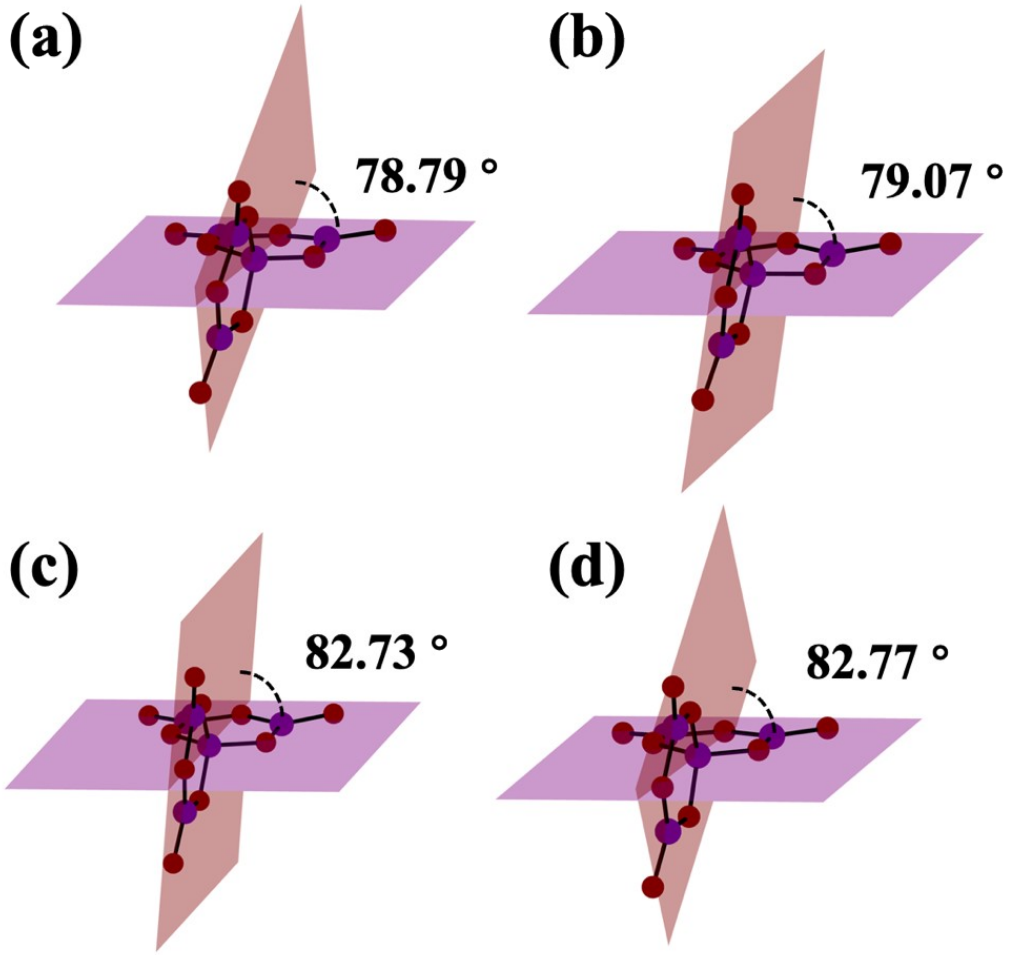

Figure S3. The dihedral angles of B_5O_{10} groups in (a) $Rb_7SrSc_2B_{15}O_{30}$, (b) $Rb_7CaSc_2B_{15}O_{30}$, (c) $Rb_7SrY_2B_{15}O_{30}$, and (d) $Rb_7SrGd_2B_{15}O_{30}$.

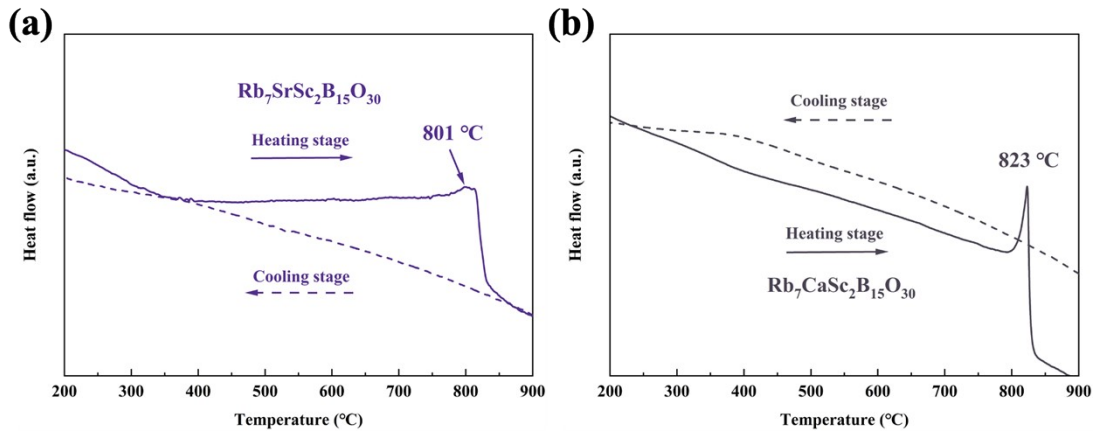

Figure S4. DCS curves of (a) $Rb_7SrSc_2B_{15}O_{30}$ and (b) $Rb_7CaSc_2B_{15}O_{30}$.

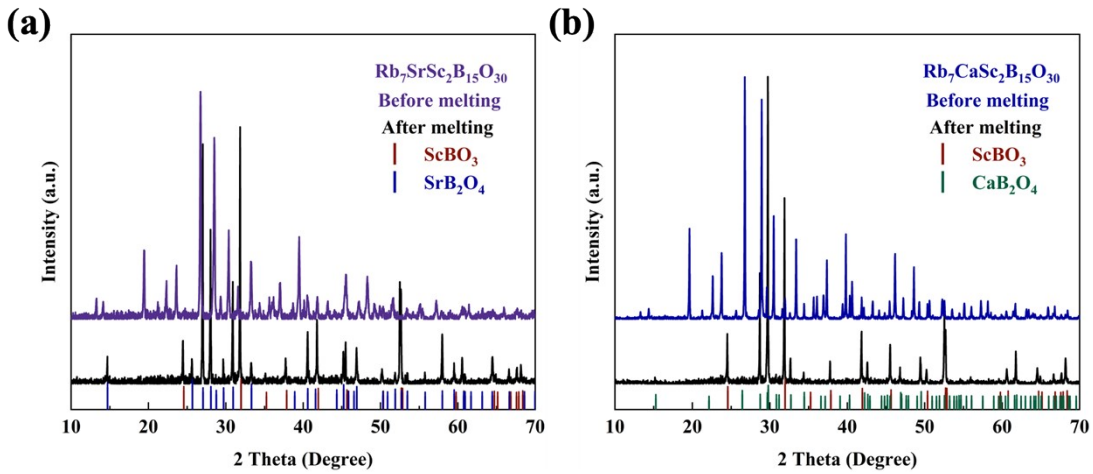

Figure S5. XRD patterns before and after melting of (a) $Rb_7SrSc_2B_{15}O_{30}$ and (b) $Rb_7CaSc_2B_{15}O_{30}$.

Table S1. Cell parameters and nonlinear optical properties of related borate compounds containing the equal fundamental building block B_5O_{10} group.

No.	Compounds	Space group	a/Å	b/Å	c/Å	Cut-off/nm	SHG response	Phase matching	Equal structure type (No.)
1	$K_3ScB_6O_{12}$[1]	*R*32	13.09	13.09	14.61	＜274	1.3×KDP	NO	3
2	$K_3YB_6O_{12}$[2]	*R*32	13.22	13.22	30.28	195	0.1×KDP	NA	4-6
3	$Rb_3YB_6O_{12}$[3]	*R*32	13.38	13.38	15.20	＜200	0.8×KDP	YES	1
4	$Rb_3NdB_6O_{12}$[4]	*R*32	13.52	13.52	31.16	197	4×α-SiO_2	NA	2, 5, 6
5	$Rb_3EuB_6O_{12}$[5]	*R*32	13.47	13.47	30.84	NA	16×α-SiO_2	NA	2, 4, 6
6	$Rb_3SmB_6O_{12}$[6]	*R*32	13.48	13.48	30.93	NA	6.5×α-SiO_2	NA	2, 4, 5
7	$K_6LiCaSc_2B_{15}O_{30}$[7]	*R*32	12.65	12.65	15.18	<200	0.4×KDP	YES	7-10
8	$K_6NaCaSc_2B_{15}O_{30}$[7]	*R*32	12.76	12.76	15.03	<200	0.4×KDP	YES	7-10
9	$K_6Li_{0.7}Na_{0.3}CaSc_2B_{15}O_{30}$[7]	*R*32	12.69	12.69	15.11	190	0.4×KDP	YES	7-10
10	$K_6NaSrSc_2B_{15}O_{30}$[1]	*R*32	12.80	12.80	15.28	＜248	0.7×KDP	YES	7-10
11	$K_6Li_3Sc_2B_{15}O_{30}$[8]	*R*32	12.71	12.71	14.91	190	1×KDP	NO	--
12	$K_7Li_2Y_2B_{15}O_{30}$[9]	*R*32	13.35	13.35	14.70	＜244	0.8×KDP	YES	--
13	$K_7CaY_2B_{15}O_{30}$[10]	*R*32	13.21	13.21	14.94	＜190	0.9×KDP	YES	13-26
14	$K_7SrY_2B_{15}O_{30}$[10]	*R*32	13.11	13.11	15.31	＜190	1.1×KDP	YES	13-26
15	$K_7BaY_2B_{15}O_{30}$[10]	*R*32	12.98	12.98	15.71	＜190	1.2×KDP	YES	13-26
16	$K_7CdGd_2B_{15}O_{30}$[11]	*R*32	13.31	13.31	14.85	＜206	1.7×KDP	YES	13-26
17	$K_7CdLu_2B_{15}O_{30}$[11]	*R*32	13.15	13.15	14.82	＜192	1.9×KDP	YES	13-26
18	$K_7CdSc_2B_{15}O_{30}$[11]	*R*32	13.11	13.11	14.62	＜200	1.5×KDP	YES	13-26
19	$K_7CdY_2B_{15}O_{30}$[11]	*R*32	13.29	13.29	14.87	＜200	1.6×KDP	YES	13-26
20	$K_7PbY_2B_{15}O_{30}$[11]	*R*32	13.10	13.10	15.32	NA	2.1×KDP	YES	13-26
21	$K_7CaBi_2B_{15}O_{30}$[12]	*R*32	13.33	13.33	14.98	＜282	0.6×KDP	YES	13-26
22	$K_7CaLa_2B_{15}O_{30}$[12]	*R*32	13.45	13.45	15.23	NA	NA	NA	13-26
23	$Rb_7SrY_2B_{15}O_{30}$[13]	*R*32	13.45	13.45	15.17	＜300	0.9×KDP	NO	13-26
24	$Rb_7SrGd_2B_{15}O_{30}$[14]	*R*32	13.49	13.49	15.32	＜225	0.5×KDP	NO	13-26
25	$Rb_7SrSc_2B_{15}O_{30}$[TW]	*R*32	13.32	13.32	14.81	＜200	0.76×KDP	NO	13-26
26	$Rb_7CaSc_2B_{15}O_{30}$[TW]	*R*32	13.31	13.31	14.59	＜200	0.88×KDP	NO	13-26
27	$K_{21}Yb_8B_{45}O_{90}$[15]	*R*32	13.20	13.20	14.76	210	1×KDP	NO	--

“NA” means that the experimental data is not applicable, and “TW” means that the compound report in this work.

Table S2. Crystallographic data and structure refinements for $Rb_7SrSc_2B_{15}O_{30}$ and $Rb_7CaSc_2B_{15}O_{30}$.

Empirical formula	$Rb_7SrSc_2B_{15}O_{30}$	$Rb_7CaSc_2B_{15}O_{30}$
Temperature/K	296.15	296.15
Crystal system	trigonal	trigonal
Space group	*R*32	*R*32
a/Å	13.3256(10)	13.3114(10)
c/Å	14.8199(16)	14.5992(16)
α/°	90	90
β/°	90	90
γ/°	120	120
Volume/Å^3	2279.0(4)	2240.3(4)
Z	3	3
ρ_{calc}g/cm^3	3.099	3.047
μ/mm^{-1}	13.439	12.077
F (000)	1962.0	1908.0
Radiation	Mo K*α* (*λ* = 0.71073)	Mo K*α* (*λ* = 0.71073)
2Θ range for data collection/°	4.474 to 55.612	4.502 to 60.928
Index ranges	-17 ≤ h ≤ 16, -16 ≤ k ≤ 15, -19 ≤ l ≤ 17	-18 ≤ h ≤ 17, -18 ≤ k ≤ 18, -20 ≤ l ≤ 12
Reflections collected	8878	9023
Independent reflections	1132 [R_{int} = 0.0973, R_{sigma} = 0.0996]	1513 [R_{int} = 0.0946, R_{sigma} = 0.1184]
Goodness-of-fit on F^2	1.062	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0611, wR_2 = 0.1575	R_1 = 0.0508, wR_2 = 0.0844
Final R indexes [all data]	R_1 = 0.1084, wR_2 = 0.1772	R_1 = 0.1145, wR_2 = 0.0974
Largest diff. peak/hole / e Å^{-3}	1.90/-2.84	0.86/-0.99
Flack parameter	0.19(6)	0.036(15)

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma wF_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$.

Table S3. Atomic coordinates and equivalent isotropic temperature factors for $Rb_7SrSc_2B_{15}O_{30}$.

Atom	***x*** **×10⁴**	***y*** **×10⁴**	***z*** **×10⁴**	**U_{eq} (Å²×10³)**
Rb1	4547(2)	10000	5000	28.9(8)
Rb2	6667	8098(2)	3333	33.6(9)
Rb3	3333	6667	6667	34.2(14)
Sr	10000	10000	5000	54.4(19)
Sc	3333	6667	3888(3)	0.7(10)
B1	5951(19)	9284(19)	6667	30(9)
B2	7500(30)	8980(20)	6040(20)	52(9)
B3	5634(17)	8032(19)	5284(15)	26(6)
O1	5281(12)	8618(12)	5870(8)	25(3)
O2	6038(12)	10406(12)	6638(11)	35(4)
O3	4917(12)	7299(13)	4672(10)	34(4)
O4	6742(10)	8235(12)	5403(12)	37(4)
O5	8626(12)	9257(16)	6070(13)	49(4)

Table S4. Atomic coordinates and equivalent isotropic temperature factors for $Rb_7CaSc_2B_{15}O_{30}$.

Atom	***x*** **×10⁴**	***y*** **×10⁴**	***z*** **×10⁴**	U_{eq} **(Å²×10³)**
Rb1	3333	1206.7(10)	6667	29.4(4)
Rb2	5242.8(11)	5242.8(11)	5000	33.1(4)
Rb3	6667	3333	8333	30.7(7)
Ca	3333	6667	6667	12.3(10)
Sc	6667	3333	5549(2)	18.2(7)
B1	4099(12)	3333	8333	17(4)
B2	5314(10)	4251(10)	6958(7)	19(3)
B3	4383(10)	5225(10)	7704(8)	24(3)
O1	4728(6)	3327(5)	7519(4)	21.9(16)
O2	3962(6)	4365(6)	8357(4)	28.7(17)
O3	5122(6)	5188(6)	7048(5)	36.9(18)
O4	4094(7)	6048(6)	7728(4)	32.0(18)
O5	6059(6)	4292(6)	6317(4)	26.7(17)

Table S5. Selected bond lengths in Å for $Rb_7SrSc_2B_{15}O_{30}$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Rb1	O1[1]	2.795(13)	Rb3	O1[2]	2.853(15)
Rb1	O1	2.795(13)	Sr	O5[6]	2.244(16)
Rb1	O2	3.009(16)	Sr	O5[13]	2.244(16)
Rb1	O2[1]	3.009(16)	Sr	O5[1]	2.244(16)
Rb1	O3[2]	2.925(16)	Sr	O5[14]	2.244(16)
Rb1	O3[3]	2.925(16)	Sr	O5	2.244(16)
Rb1	O4[2]	3.269(14)	Sr	O5[15]	2.244(16)
Rb1	O4[3]	3.269(14)	Sc	O3[2]	2.176(15)
Rb2	O2[1]	2.937(15)	Sc	O3	2.176(15)
Rb2	O2[4]	2.937(15)	Sc	O3[9]	2.176(15)
Rb2	O3	2.833(14)	Sc	O5[7]	2.331(18)
Rb2	O3[5]	2.833(14)	Sc	O5[12]	2.331(18)
Rb2	O4	3.071(17)	Sc	O5[4]	2.331(18)
Rb2	O4[5]	3.071(17)	B1	O1	1.479(18)
Rb2	O5[6]	3.28(2)	B1	O2	1.441(17)
Rb2	O5[7]	3.28(2)	B2	O4	1.38(2)
Rb3	O1[8]	2.853(15)	B2	O5	1.36(3)
Rb3	O1[9]	2.853(15)	B2	O2[10]	1.35(3)
Rb3	O1[10]	2.853(15)	B3	O1	1.40(3)
Rb3	O1	2.853(15)	B3	O3	1.33(2)
Rb3	O1[11]	2.853(15)	B3	O4	1.37(2)

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

Table S6. Selected bond lengths in Å for $Rb_7CaSc_2B_{15}O_{30}$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Rb1	O1[4]	2.779(6)	Rb3	O1	2.838(7)
Rb1	O1	2.779(6)	Ca	O4[8]	2.222(6)
Rb1	O2[5]	2.992(7)	Ca	O4[4]	2.222(6)
Rb1	O2[1]	2.992(7)	Ca	O4[15]	2.222(6)
Rb1	O3[3]	3.223(7)	Ca	O4[14]	2.222(6)
Rb1	O3[2]	3.223(7)	Ca	O4	2.222(6)
Rb1	O5[3]	2.907(7)	Ca	O4[13]	2.222(6)
Rb1	O5[2]	2.907(7)	Sc	O4[16]	2.319(7)
Rb2	O2[4]	2.943(7)	Sc	O4[1]	2.319(7)
Rb2	O2[1]	2.943(7)	Sc	O4[7]	2.319(7)
Rb2	O3[6]	2.993(7)	Sc	O5[9]	2.138(6)
Rb2	O3	2.993(7)	Sc	O5[3]	2.138(6)
Rb2	O4[7]	3.255(8)	Sc	O5	2.138(6)
Rb2	O4[8]	3.255(8)	B1	O1	1.456(10)
Rb2	O5	2.803(6)	B1	O2	1.474(11)
Rb2	O5[6]	2.803(6)	B2	O1	1.354(12)
Rb3	O1[3]	2.838(7)	B2	O3	1.399(12)
Rb3	O1[5]	2.838(7)	B2	O5	1.345(12)
Rb3	O1[10]	2.838(7)	B3	O2	1.374(12)
Rb3	O1[11]	2.838(7)	B3	O3	1.392(12)
Rb3	O1[9]	2.838(7)	B3	O4	1.331(12)

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

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