Supplementary Information

$Rb_3BaTeB_7O_{15}$: A Novel $[B_7O_{16}]$ Fundamental Building Block in a New Telluroborate with $[TeO_3]$ Polyhedra

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Table S1. The final Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Rb_3BaTeB_7O_{15}$, U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor, and the Bond Valence Sum (BVS) for each atom in the asymmetric unit.

Atom	x	y	z	U(eq)	BVS
Rb(1)	3376(1)	7088(1)	7392(1)	25(1)	1.06
Rb(2)	9154(1)	3232(1)	6340(1)	21(1)	1.08
Rb(3)	8619(1)	7538(1)	4969(1)	20(1)	1.05
Ba(1)	6060(1)	7840(1)	6275(1)	11(1)	2.20
Te(1)	6396(1)	2607(1)	5183(1)	13(1)	4.21
B(1)	7445(6)	6260(9)	7697(2)	10(1)	3.07
B(2)	9102(6)	8103(9)	7170(2)	10(1)	3.02
B(3)	10498(6)	8206(9)	6380(2)	9(1)	3.04
B(4)	12654(6)	10620(9)	6317(2)	11(1)	3.03
B(5)	14915(7)	12036(9)	6924(2)	12(1)	3.01
B(6)	6588(6)	5728(9)	3727(2)	9(1)	3.12
B(7)	12164(7)	7501(9)	5746(2)	10(1)	3.05
O(1)	8079(4)	3004(6)	4825(1)	15(1)	2.25
O(2)	9295(4)	7645(5)	6621(1)	12(1)	2.07
O(3)	11403(4)	9791(5)	6584(1)	13(1)	2.07
O(4)	12707(4)	9599(5)	5816(1)	11(1)	1.88
O(5)	6746(4)	4931(6)	5592(2)	22(1)	2.12
O(6)	7149(4)	505(6)	5616(2)	21(1)	2.12
O(7)	8498(4)	6424(5)	8116(1)	11(1)	2.07
O(8)	7650(4)	7073(6)	7225(1)	14(1)	2.04
O(9)	10749(4)	7136(5)	5946(1)	11(1)	2.05
O(10)	14013(4)	10371(5)	6675(1)	12(1)	2.09
O(11)	6095(4)	5398(5)	7757(1)	13(1)	2.11
O(12)	13341(4)	6114(6)	6008(2)	20(1)	2.09
O(13)	10286(4)	7281(5)	7529(1)	11(1)	1.93
O(14)	5357(4)	5970(5)	3375(1)	14(1)	2.01
O(15)	7691(4)	7147(5)	3796(2)	15(1)	2.07

Table S2. Selected bond distances (Å) and angles (deg) for $Rb_3BaTeB_7O_{15}$.

Ba(1)-O(6)#1	2.686(4)	O(7)#3-Ba(1)-O(4)#2	88.94(9)
Ba(1)-O(5)	2.693(4)	O(14)#4-Ba(1)-O(4)#2	88.42(9)
Ba(1)-O(12)#2	2.719(4)	O(2)-Ba(1)-O(4)#2	162.02(9)
Ba(1)-O(8)	2.728(4)	O(6)-Te(1)-O(5)	102.91(18)
Ba(1)-O(10)#2	2.766(3)	O(6)-Te(1)-O(1)	97.65(17)
Ba(1)-O(7)#3	2.784(4)	O(5)-Te(1)-O(1)	94.48(16)
Ba(1)-O(14)#4	2.955(3)	O(11)-Rb(1)-O(13)#2	145.42(10)
Ba(1)-O(2)	2.969(4)	O(11)-Rb(1)-O(10)#2	104.99(10)
Ba(1)-O(4)#2	3.327(4)	O(13)#2-Rb(1)-O(10)#2	108.88(10)
Te(1)-O(6)	1.828(4)	O(11)-Rb(1)-O(3)#6	63.28(10)
Te(1)-O(5)	1.830(4)	O(13)#2-Rb(1)-O(3)#6	82.59(9)
Te(1)-O(1)	1.903(3)	O(10)#2-Rb(1)-O(3)#6	156.35(10)
Rb(1)-O(11)	2.756(3)	O(11)-Rb(1)-O(3)#2	150.17(10)
Rb(1)-O(13)#2	2.881(3)	O(13)#2-Rb(1)-O(3)#2	64.36(9)
Rb(1)-O(10)#2	2.908(4)	O(10)#2-Rb(1)-O(3)#2	46.67(9)
Rb(1)-O(3)#6	3.008(4)	O(3)#6-Rb(1)-O(3)#2	146.29(4)
Rb(1)-O(3)#2	3.101(4)	O(11)-Rb(1)-O(14)#4	65.16(10)
Rb(1)-O(14)#4	3.109(4)	O(13)#2-Rb(1)-O(14)#4	123.49(10)
Rb(1)-O(13)#6	3.310(3)	O(10)#2-Rb(1)-O(14)#4	86.06(10)
Rb(1)-O(13)#3	3.541(4)	O(3)#6-Rb(1)-O(14)#4	105.14(9)
Rb(2)-O(2)	2.918(3)	O(3)#2-Rb(1)-O(14)#4	98.90(9)
Rb(2)-O(5)	2.940(4)	O(11)-Rb(1)-O(13)#6	46.00(9)
Rb(2)-O(15)#7	2.947(4)	O(13)#2-Rb(1)-O(13)#6	112.94(10)
Rb(2)-O(11)#6	2.986(4)	O(10)#2-Rb(1)-O(13)#6	127.67(9)
Rb(2)-O(6)	3.001(4)	O(3)#6-Rb(1)-O(13)#6	60.46(9)
Rb(2)-O(3)#5	3.021(4)	O(3)#2-Rb(1)-O(13)#6	137.63(9)
Rb(2)-O(9)	3.126(3)	O(14)#4-Rb(1)-O(13)#6	44.69(9)
Rb(2)-O(7)#6	3.161(3)	O(11)-Rb(1)-O(13)#3	93.57(9)
Rb(3)-O(4)#8	2.884(4)	O(13)#2-Rb(1)-O(13)#3	106.65(10)
Rb(3)-O(6)#1	2.959(4)	O(10)#2-Rb(1)-O(13)#3	42.43(9)
Rb(3)-O(1)	2.962(4)	O(3)#6-Rb(1)-O(13)#3	115.16(9)
Rb(3)-O(9)	2.989(4)	O(3)#2-Rb(1)-O(13)#3	71.30(9)
Rb(3)-O(5)	2.994(4)	O(14)#4-Rb(1)-O(13)#3	118.46(9)
Rb(3)-O(1)#7	3.005(4)	O(13)#6-Rb(1)-O(13)#3	138.60(11)
Rb(3)-O(15)	3.048(4)	O(2)-Rb(2)-O(5)	79.03(10)
Rb(3)-O(1)#1	3.551(4)	O(2)-Rb(2)-O(15)#7	95.54(10)
B(1)-O(7)	1.355(7)	O(5)-Rb(2)-O(15)#7	127.50(10)
B(1)-O(8)	1.358(6)	O(2)-Rb(2)-O(11)#6	113.65(10)
B(1)-O(11)	1.374(6)	O(5)-Rb(2)-O(11)#6	127.88(10)
B(2)-O(13)	1.430(7)	O(15)#7-Rb(2)-O(11)#6	102.37(10)
B(2)-O(2)	1.477(7)	O(2)-Rb(2)-O(6)	136.31(10)
B(2)-O(11)#3	1.496(6)	O(5)-Rb(2)-O(6)	57.55(10)
B(2)-O(8)	1.500(7)	O(15)#7-Rb(2)-O(6)	113.75(10)

B(3)-O(9)	1.355(7)	O(11)#6-Rb(2)-O(6)	91.77(10)
B(3)-O(3)	1.371(6)	O(2)-Rb(2)-O(3)#5	130.43(10)
B(3)-O(2)	1.374(6)	O(5)-Rb(2)-O(3)#5	146.77(10)
B(4)-O(4)	1.454(7)	O(15)#7-Rb(2)-O(3)#5	47.15(9)
B(4)-O(10)	1.455(7)	O(11)#6-Rb(2)-O(3)#5	60.62(9)
B(4)-O(15)#8	1.486(6)	O(6)-Rb(2)-O(3)#5	92.70(10)
B(4)-O(3)	1.502(6)	O(2)-Rb(2)-O(9)	45.36(9)
B(5)-O(10)	1.447(7)	O(5)-Rb(2)-O(9)	80.10(10)
B(5)-O(13)#10	1.455(7)	O(15)#7-Rb(2)-O(9)	61.82(9)
B(5)-O(14)#8	1.497(7)	O(11)#6-Rb(2)-O(9)	145.57(10)
B(5)-O(7)#10	1.513(6)	O(6)-Rb(2)-O(9)	122.33(10)
B(6)-O(15)	1.349(6)	O(3)#5-Rb(2)-O(9)	108.79(9)
B(6)-O(14)	1.358(7)	O(2)-Rb(2)-O(7)#6	104.89(9)
B(6)-O(12)#7	1.363(7)	O(5)-Rb(2)-O(7)#6	83.10(10)
B(7)-O(4)	1.436(6)	O(15)#7-Rb(2)-O(7)#6	146.41(9)
B(7)-O(9)	1.466(7)	O(11)#6-Rb(2)-O(7)#6	45.01(9)
B(7)-O(12)	1.486(7)	O(6)-Rb(2)-O(7)#6	67.94(10)
B(7)-O(1)#7	1.498(7)	O(3)#5-Rb(2)-O(7)#6	100.09(9)
O(6)#1-Ba(1)-O(5)	83.76(12)	O(9)-Rb(2)-O(7)#6	148.15(9)
O(6)#1-Ba(1)-O(12)#2	119.67(12)	O(4)#8-Rb(3)-O(6)#1	78.95(10)
O(5)-Ba(1)-O(12)#2	80.29(12)	O(4)#8-Rb(3)-O(1)	119.19(10)
O(6)#1-Ba(1)-O(8)	119.12(12)	O(6)#1-Rb(3)-O(1)	128.41(10)
O(5)-Ba(1)-O(8)	108.83(12)	O(4)#8-Rb(3)-O(9)	144.72(9)
O(12)#2-Ba(1)-O(8)	121.13(11)	O(6)#1-Rb(3)-O(9)	82.60(10)
O(6)#1-Ba(1)-O(10)#2	100.53(11)	O(1)-Rb(3)-O(9)	95.81(10)
O(5)-Ba(1)-O(10)#2	150.79(11)	O(4)#8-Rb(3)-O(5)	121.05(11)
O(12)#2-Ba(1)-O(10)#2	72.46(11)	O(6)#1-Rb(3)-O(5)	74.18(10)
O(8)-Ba(1)-O(10)#2	94.39(10)	O(1)-Rb(3)-O(5)	54.80(10)
O(6)#1-Ba(1)-O(7)#3	78.09(11)	O(9)-Rb(3)-O(5)	81.52(10)
O(5)-Ba(1)-O(7)#3	155.76(11)	O(4)#8-Rb(3)-O(1)#7	121.20(10)
O(12)#2-Ba(1)-O(7)#3	122.75(11)	O(6)#1-Rb(3)-O(1)#7	119.23(10)
O(8)-Ba(1)-O(7)#3	67.62(10)	O(1)-Rb(3)-O(1)#7	93.17(9)
O(10)#2-Ba(1)-O(7)#3	50.34(10)	O(9)-Rb(3)-O(1)#7	46.70(9)
O(6)#1-Ba(1)-O(14)#4	158.25(11)	O(5)-Rb(3)-O(1)#7	117.74(11)
O(5)-Ba(1)-O(14)#4	76.95(11)	O(4)#8-Rb(3)-O(15)	46.80(9)
O(12)#2-Ba(1)-O(14)#4	47.38(10)	O(6)#1-Rb(3)-O(15)	121.63(10)
O(8)-Ba(1)-O(14)#4	77.26(10)	O(1)-Rb(3)-O(15)	76.93(10)
O(10)#2-Ba(1)-O(14)#4	91.73(10)	O(9)-Rb(3)-O(15)	153.99(9)
O(7)#3-Ba(1)-O(14)#4	123.18(10)	O(5)-Rb(3)-O(15)	112.42(10)
O(6)#1-Ba(1)-O(2)	77.62(11)	O(1)#7-Rb(3)-O(15)	108.13(10)
O(5)-Ba(1)-O(2)	82.20(11)	O(4)#8-Rb(3)-O(1)#1	42.11(9)
O(12)#2-Ba(1)-O(2)	153.55(10)	O(6)#1-Rb(3)-O(1)#1	50.11(9)
O(8)-Ba(1)-O(2)	47.89(10)	O(1)-Rb(3)-O(1)#1	159.37(14)
O(10)#2-Ba(1)-O(2)	127.00(10)	O(9)-Rb(3)-O(1)#1	103.87(9)

O(7)#3-Ba(1)-O(2)	78.35(9)	O(5)-Rb(3)-O(1)#1	121.73(9)
O(14)#4-Ba(1)-O(2)	109.15(9)	O(1)#7-Rb(3)-O(1)#1	104.76(8)
O(6)#1-Ba(1)-O(4)#2	87.41(10)	O(15)-Rb(3)-O(1)#1	87.68(9)
O(5)-Ba(1)-O(4)#2	106.27(11)	O(7)-B(1)-O(8)	121.4(5)
O(12)#2-Ba(1)-O(4)#2	44.20(10)	O(7)-B(1)-O(11)	119.6(5)
O(8)-Ba(1)-O(4)#2	137.62(9)	O(8)-B(1)-O(11)	118.8(5)
O(10)#2-Ba(1)-O(4)#2	45.81(9)	O(13)-B(2)-O(2)	112.1(4)
O(4)-B(4)-O(3)	111.2(4)	O(13)-B(2)-O(11)#3	111.8(4)
O(10)-B(4)-O(3)	107.7(4)	O(2)-B(2)-O(11)#3	110.4(4)
O(15)#8-B(4)-O(3)	106.1(4)	O(13)-B(2)-O(8)	112.1(4)
O(10)-B(5)-O(13)#9	112.1(4)	O(2)-B(2)-O(8)	102.5(4)
O(10)-B(5)-O(14)#8	110.7(5)	O(11)#3-B(2)-O(8)	107.4(4)
O(13)#10-B(5)-O(14)#8	112.0(4)	O(9)-B(3)-O(3)	122.5(5)
O(10)-B(5)-O(7)#10	105.8(4)	O(9)-B(3)-O(2)	117.9(5)
O(13)#10-B(5)-O(7)#9	109.4(4)	O(3)-B(3)-O(2)	119.6(5)
O(14)#8-B(5)-O(7)#9	106.5(4)	O(4)-B(4)-O(10)	113.1(4)
O(15)-B(6)-O(14)	123.2(5)	O(4)-B(4)-O(15)#8	106.8(4)
O(15)-B(6)-O(12)#7	122.0(5)	O(10)-B(4)-O(15)#8	111.8(4)
O(14)-B(6)-O(12)#7	114.7(5)	O(9)-B(7)-O(12)	111.1(4)
O(4)-B(7)-O(9)	114.1(4)	O(4)-B(7)-O(1)#7	109.4(4)
O(4)-B(7)-O(12)	106.6(4)	O(9)-B(7)-O(1)#7	106.5(4)
O(12)-B(7)-O(1)#7	109.0(4)		

Symmetry transformations used to generate equivalent atoms:
#1 x, y+1, z
#2 x-1, y, z
#3 -x+3/2, y+1/2, -z+3/2
#4 -x+1, -y+1, -z+1
#5 x, y-1, z
#6 -x+3/2, y-1/2, -z+3/2
#7 -x+2, -y+1, -z+1
#8 -x+2, -y+2, -z+1
#9 -x+5/2, y+1/2, -z+3/2

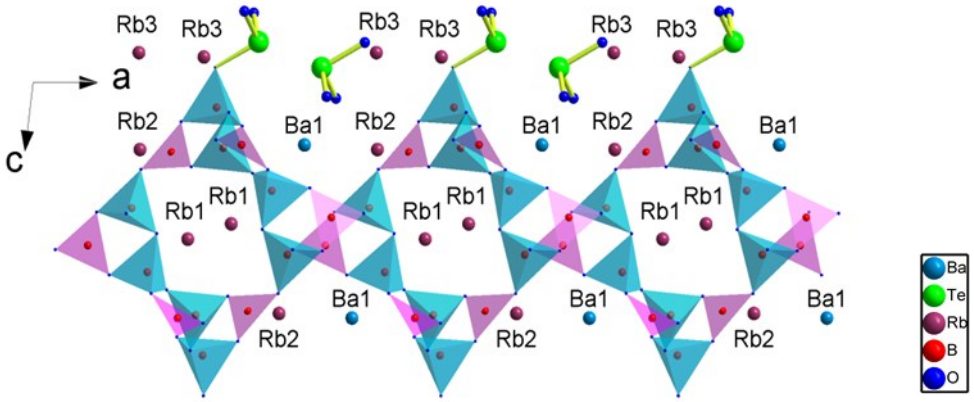

Figure S1. Coordination environment for three types of the Rb atoms.

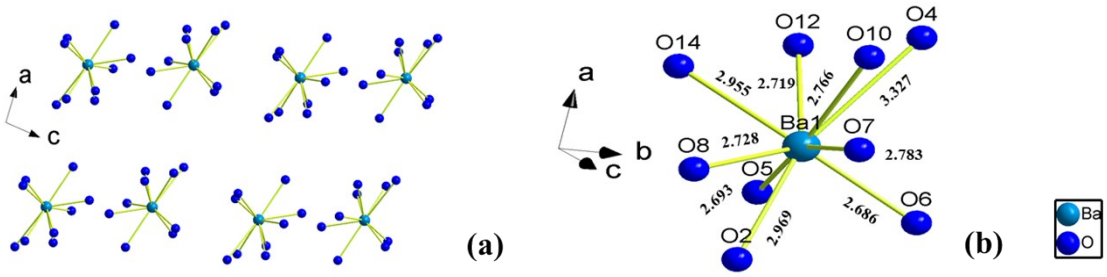

Figure S2. (a) The arrangement of the [BaO_9] groups; (b) Coordination environment of the Ba atom.

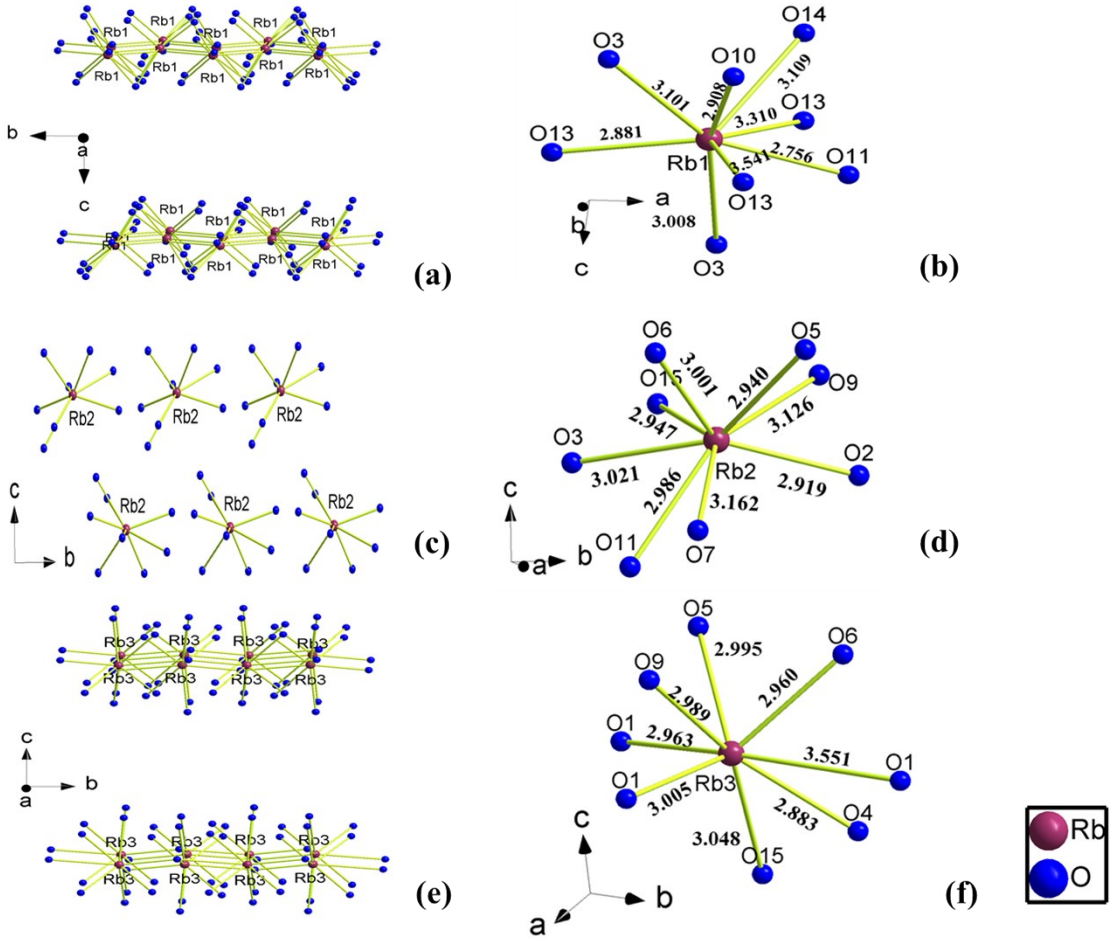

Figure S3. (a) (c) (e) The arrangement of the [RbO_8] groups; (b) (d) (f) Coordination environment of the Rb atoms.

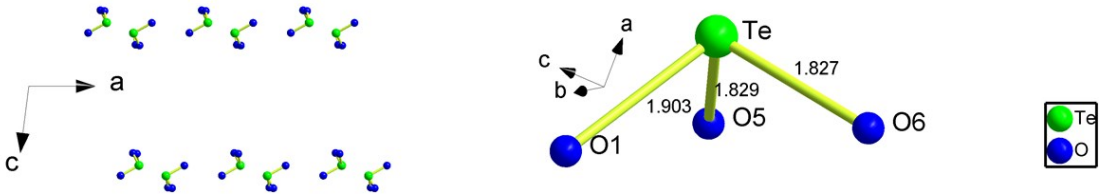

Figure S4. The arrangement of the [TeO_3] groups and coordination environment of the Te atom.

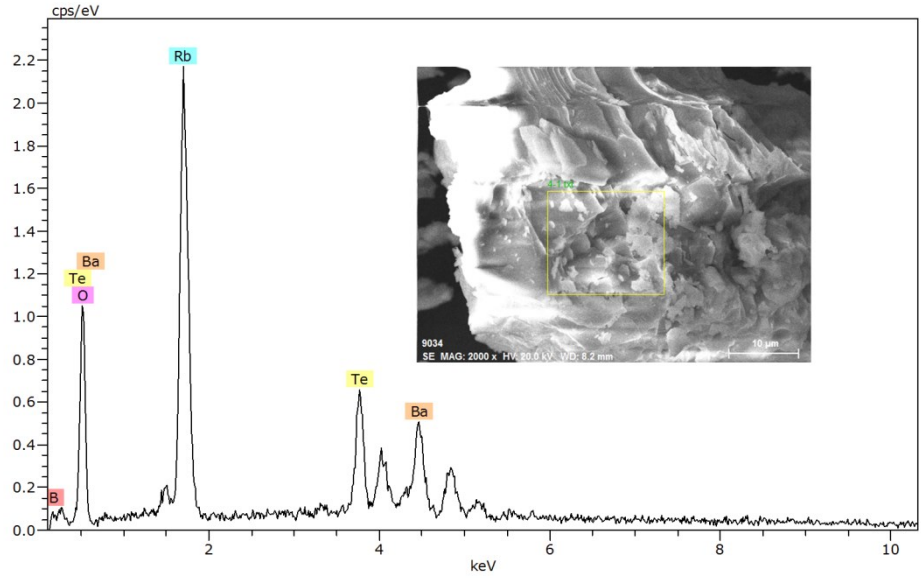

Figure S5. Energy-dispersive X-ray spectroscopy of $Rb_3BaTeB_7O_{15}$.