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Synthesis, Crystal Structures, and Electronic Properties of One Dimensional $Ba_9Sn_3(Te_{1-x}Se_x)_{15}$ (x=0-1)

Jun Zhang[a], Rui Su[b], Xiancheng Wang*[a], Wenmin Li[a], Jianfa Zhao[a], Zheng Deng[a], Sijia Zhang[a], Shaomin Feng[a], Qingqing Liu[a], Huaizhou Zhao[a], Pengfei Guan*[b] and ChangqingJin*[a,c,d]

[a] Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190 & University of Chinese Academy of Sciences, Beijing 100049, China.

[b] Beijing Computational Science Research Center, Beijing 100193, China

[c] Collaborative Innovation Center of Quantum Matter, Beijing 100190, China

[d] School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

Table SI-SIV presents the results of refinement of single crystal X-ray diffraction for $Ba_9Sn_3Te_{15}$. Table SV-SIX shows the crystallographic data for $Ba_9Sn_3(Te_{1-x}Se_x)_{15}$ (x = 0.2, 0.4, 0.6, 0.8 and 1) refined from powder X-ray diffractions, respectively. Fig. S1-S5 presents the powder X-ray diffraction and their refinement for $Ba_9Sn_3(Te_{1-x}Se_x)_{15}$ (x = 0.2, 0.4, 0.6, 0.8 and 1), respectively. From the Table SV-SIX, we can see that the doped Se atoms favor to firstly occupy the Te1 and Te2 sites. When increasing the doping level of Se, the sites from Te3 to Te6 would be occupied successively.

Table SI. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for $Ba_9Sn_3Te_{15}$. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	wyck.	***x***	***y***	***z***	Occ.	**U(eq)**
Ba1	12l	0.3774 (0)	0.3876 (2)	0.0833 (2)	1	16.7(2)
Ba2	6k	-0.0222 (9)	0.3690 (9)	0.2500	1	14.9(3)
Sn1	2a	0	0	0	1	19.3(6)
Sn2	4g	0	0	0.1661 (6)	0.96(4)	14.5(5)
Te1	12l	-0.0027 (4)	0.2497 (0)	0.0837 (5)	1	15.03(18)
Te2	6k	0.2447 (0)	0.2574 (4)	0.2500	1	12.9(2)
Te3	2c	0.3333	0.6667	0	1	15.7(4)
Te4	4h	0.3333	0.6667	0.1830 (3)	1	11.1(3)
Te5	4i	-0.3333	0.3333	0.1559 (9)	1	18.2(4)
Te6	4i	-0.3333	0.3333	0.0081(6)	0.5	13(2)

Table SII. Anisotropic Displacement Parameters (Å^2×10^3) for $Ba_9Sn_3Te_{15}$. 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_{23}	U_{13}	U_{12}
Ba1	14.5(5)	16.3(4)	18.4(3)	1.4(3)	-1.3(3)	7.1(3)
Ba2	11.9(5)	13.5(6)	18.6(4)	0	0	5.8(5)
Te1	16.0(4)	16.3(6)	15.5(3)	0.2(3)	-0.2(2)	10.2(6)
Te2	11.3(7)	13.3(6)	15.8(5)	0	0	7.4(5)
Te3	12.0(6)	12.0(6)	23(1)	0	0	6.0(3)
Te4	11.9(4)	11.9(4)	9.3(5)	0	0	6.0(2)
Te5	12.3(5)	12.3(5)	30.2(11)	0	0	6.1(3)
Te6	12.5(8)	12.5(8)	15(6)	0	0	6.3(4)
Sn1	17.5(8)	17.5(8)	23.1(16)	0	0	8.7(4)
Sn2	16.3(6)	16.3(6)	10.9(8)	0	0	8.1(3)

Table SIII. Bond Lengths for $Ba_9Sn_3Te_{15}$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ba1	Ba1[1]	4.2156(14)	Te2	Sn2	3.1074(18)
Ba1	Ba2[2]	4.2395(9)	Te3	Ba1[8]	3.5572(12)
Ba1	Te1[2]	3.7540(11)	Te3	Ba1[3]	3.5572(12)
Ba1	Te1[3]	3.7239(10)	Te3	Ba1[1]	3.5572(12)
Ba1	Te1	3.4132(16)	Te3	Ba1[2]	3.5572(12)
Ba1	Te1[4]	3.4826(16)	Te3	Ba1[13]	3.5572(12)
Ba1	Te2	3.7148(9)	Te4	Ba1[8]	3.7347(13)
Ba1	Te3	3.5572(12)	Te4	Ba1[2]	3.7348(13)
Ba1	Te4	3.7348(13)	Te4	Ba2[2]	3.6587(12)
Ba1	Te5[5]	3.6068(14)	Te4	Ba2[7]	3.6587(12)
Ba1	Te6[6]	3.787(7)	Te4	Te4[7]	2.782(3)
Ba1	Te6[5]	3.629(6)	Te5	Ba1[14]	3.6067(14)
Ba2	Ba1[7]	4.2395(9)	Te5	Ba1[10]	3.6068(14)
Ba2	Ba1[8]	4.2395(9)	Te5	Ba1[8]	3.6068(14)
Ba2	Te1	3.7021(9)	Te5	Ba2[11]	3.5953(15)
Ba2	Te1[9]	3.7021(9)	Te5	Ba2[15]	3.5953(15)
Ba2	Te2[10]	3.4163(16)	Te5	Te6	3.071(13)
Ba2	Te2	3.4509(19)	Te6	Ba1[14]	3.629(6)
Ba2	Te2[7]	3.7883(18)	Te6	Ba1[16]	3.787(7)
Ba2	Te4	3.6587(12)	Te6	Ba1[3]	3.787(7)

Ba2	Te4^{7}	3.6587(12)	Te6	Ba1^{10}	3.629(6)
Ba2	Te5	3.5953(15)	Te6	Ba1^{8}	3.629(6)
Ba2	Te5^{11}	3.5954(15)	Te6	Ba1^{17}	3.787(7)
Te1	Ba1^{8}	3.7540(11)	Sn1	Te1^{18}	3.1044(8)
Te1	Ba1^{10}	3.4825(16)	Sn1	Te1^{19}	3.1044(8)
Te1	Ba1^{3}	3.7239(10)	Sn1	Te1^{10}	3.1044(8)
Te1	Sn1	3.1044(8)	Sn1	Te1^{3}	3.1044(8)
Te1	Sn2	3.0889(16)	Sn1	Te1^{4}	3.1044(8)
Te2	Ba1^{9}	3.7148(9)	Sn2	Te1^{10}	3.0890(16)
Te2	Ba2^{2}	3.7883(18)	Sn2	Te1^{4}	3.0890(16)
Te2	Ba2^{12}	3.4163(16)	Sn2	Te2^{10}	3.1074(18)
Te2	Sn2^{12}	3.1074(18)	Sn2	Te2^{12}	3.1074(18)

^{1}1-Y,1-X,-Z; ^{2}1-Y,1+X-Y,+Z; ^{3}+Y-X,+Y,-Z; ^{4}+Y-X,-X,+Z; ^{5}1+X,+Y,+Z; ^{6}1-Y,-X,-Z; ^{7}+Y-X,1-X,1/2-Z; ^{8}+Y-X,1-X,+Z; ^{9}+X,+Y,1/2-Z; ^{10}-Y,+X-Y,+Z; ^{11}-1+Y-X,-X,1/2-Z; ^{12}+Y-X,-X,1/2-Z; ^{13}+X,1+X-Y,-Z; ^{14}-1+X,+Y,+Z; ^{15}-Y,1+X-Y,+Z; ^{16}-1+X,+X-Y,-Z; ^{17}-Y,1-X,-Z; ^{18}+X,+X-Y,-Z; ^{19}-Y,-X,-Z

Table SIV. Bond Angles for $Ba_9Sn_3Te_{15}$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Ba1^{1}	Ba1	Ba2^{2}	110.09(2)	Sn2	Te1	Ba1^{10}	81.02(3)
Te1^{2}	Ba1	Ba1^{1}	55.35(2)	Sn2	Te1	Ba1	82.15(3)
Te1	Ba1	Ba1^{1}	116.47(3)	Sn2	Te1	Ba1^{8}	146.41(4)
Te1^{3}	Ba1	Ba1^{1}	56.02(2)	Sn2	Te1	Ba1^{3}	144.79(4)
Te1^{4}	Ba1	Ba1^{1}	115.47(3)	Sn2	Te1	Ba2	77.34(5)
Te1^{4}	Ba1	Ba2^{2}	112.49(3)	Sn2	Te1	Sn1	67.74(4)
Te1	Ba1	Ba2^{2}	119.08(3)	Ba1^{9}	Te2	Ba1	137.51(5)
Te1^{3}	Ba1	Ba2^{2}	165.03(2)	Ba1^{9}	Te2	Ba2^{2}	68.80(2)
Te1^{2}	Ba1	Ba2^{2}	54.772(18)	Ba1	Te2	Ba2^{2}	68.80(2)
Te1	Ba1	Te1^{3}	74.99(3)	Ba2	Te2	Ba1	95.13(3)
Te1^{4}	Ba1	Te1^{3}	73.20(3)	Ba2^{12}	Te2	Ba1^{9}	92.41(4)
Te1^{3}	Ba1	Te1^{2}	111.26(2)	Ba2	Te2	Ba1^{9}	95.13(3)
Te1^{4}	Ba1	Te1^{2}	136.80(5)	Ba2^{12}	Te2	Ba1	92.41(4)
Te1	Ba1	Te1^{4}	80.45(3)	Ba2	Te2	Ba2^{2}	108.03(5)
Te1	Ba1	Te1^{2}	142.75(5)	Ba2^{12}	Te2	Ba2^{2}	92.91(5)
Te1^{4}	Ba1	Te2	74.34(3)	Ba2^{12}	Te2	Ba2	159.06(5)
Te1	Ba1	Te2	73.27(3)	Sn2	Te2	Ba1	77.13(4)
Te1^{4}	Ba1	Te3	142.00(3)	Sn2^{12}	Te2	Ba1^{9}	77.13(4)
Te1	Ba1	Te3	75.95(3)	Sn2	Te2	Ba1^{9}	145.28(5)
Te1^{3}	Ba1	Te4	131.06(5)	Sn2^{12}	Te2	Ba1	145.28(5)

Te1^{4}	Ba1	Te4	138.41(3)
Te1	Ba1	Te4	76.47(3)
Te1	Ba1	Te5^{5}	142.16(3)
Te1^{4}	Ba1	Te5^{5}	71.93(3)
Te1^{4}	Ba1	Te6^{5}	72.18(4)
Te1^{4}	Ba1	Te6^{6}	72.96(4)
Te1	Ba1	Te6^{6}	138.99(12)
Te1^{2}	Ba1	Te6^{6}	70.06(4)
Te1	Ba1	Te6^{5}	141.92(12)
Te1^{3}	Ba1	Te6^{6}	67.82(16)
Te2	Ba1	Ba1^{1}	166.43(4)
Te2	Ba1	Ba2^{2}	56.42(3)
Te2	Ba1	Te1^{3}	137.54(3)
Te2	Ba1	Te1^{2}	111.11(3)
Te2	Ba1	Te4	66.12(3)
Te2	Ba1	Te6^{6}	125.98(16)
Te3	Ba1	Ba1^{1}	53.663(15)
Te3	Ba1	Ba2^{2}	104.969(19)
Te3	Ba1	Te1^{2}	71.80(3)
Te3	Ba1	Te1^{3}	72.16(3)
Te3	Ba1	Te2	124.83(4)
Te3	Ba1	Te4	62.79(3)
Te3	Ba1	Te5^{5}	140.47(2)
Te3	Ba1	Te6^{6}	107.25(13)
Te3	Ba1	Te6^{5}	110.78(14)
Te4	Ba1	Ba1^{1}	105.75(2)
Te4	Ba1	Ba2^{2}	54.17(2)
Te4	Ba1	Te1^{2}	72.55(3)
Te4	Ba1	Te6^{6}	142.48(6)
Te5^{5}	Ba1	Ba1^{1}	98.81(3)
Te5^{5}	Ba1	Ba2^{2}	53.81(3)
Te5^{5}	Ba1	Te1^{3}	118.98(5)
Te5^{5}	Ba1	Te1^{2}	68.88(2)
Te5^{5}	Ba1	Te2	74.68(4)
Te5^{5}	Ba1	Te4	107.97(3)
Te5^{5}	Ba1	Te6^{6}	54.85(17)
Te5^{5}	Ba1	Te6^{5}	50.23(19)
Te6^{6}	Ba1	Ba1^{1}	53.61(13)
Te6^{5}	Ba1	Ba1^{1}	57.14(14)
Te6^{5}	Ba1	Ba2^{2}	95.99(16)
Sn2^{12}	Te2	Ba2	81.06(3)
Sn2	Te2	Ba2^{12}	81.62(3)
Sn2	Te2	Ba2	81.06(3)
Sn2^{12}	Te2	Ba2^{2}	145.25(4)
Sn2	Te2	Ba2^{2}	145.25(4)
Sn2^{12}	Te2	Ba2^{12}	81.62(3)
Sn2^{12}	Te2	Sn2	68.17(7)
Ba1^{8}	Te3	Ba1	98.333(19)
Ba1^{3}	Te3	Ba1^{2}	167.39(3)
Ba1^{2}	Te3	Ba1^{1}	91.84(2)
Ba1^{2}	Te3	Ba1	98.333(19)
Ba1^{13}	Te3	Ba1^{2}	72.68(3)
Ba1^{3}	Te3	Ba1	91.84(2)
Ba1^{8}	Te3	Ba1^{1}	167.38(3)
Ba1	Te3	Ba1^{1}	72.67(3)
Ba1^{13}	Te3	Ba1	167.39(3)
Ba1^{8}	Te3	Ba1^{2}	98.334(19)
Ba1^{3}	Te3	Ba1^{1}	98.333(19)
Ba1^{8}	Te3	Ba1^{3}	72.68(3)
Ba1^{13}	Te3	Ba1^{8}	91.84(2)
Ba1^{13}	Te3	Ba1^{1}	98.334(19)
Ba1^{13}	Te3	Ba1^{3}	98.334(19)
Ba1^{2}	Te4	Ba1	92.22(3)
Ba1^{8}	Te4	Ba1^{2}	92.22(3)
Ba1^{8}	Te4	Ba1	92.21(3)
Ba2^{2}	Te4	Ba1^{8}	161.95(3)
Ba2	Te4	Ba1^{2}	161.95(3)
Ba2^{2}	Te4	Ba1^{2}	91.394(16)
Ba2^{7}	Te4	Ba1^{2}	69.97(2)
Ba2^{2}	Te4	Ba1	69.97(2)
Ba2^{7}	Te4	Ba1	161.95(3)
Ba2	Te4	Ba1^{8}	69.97(2)
Ba2^{7}	Te4	Ba1^{8}	91.395(16)
Ba2	Te4	Ba1	91.395(16)
Ba2	Te4	Ba2^{2}	106.45(2)
Ba2^{7}	Te4	Ba2^{2}	106.45(2)
Ba2^{7}	Te4	Ba2	106.45(2)
Te4^{7}	Te4	Ba1^{2}	123.68(2)
Te4^{7}	Te4	Ba1	123.68(2)
Te4^{7}	Te4	Ba1^{8}	123.68(2)

Te6^{6}	Ba1	Ba2^{2}	99.96(15)
Te6^{5}	Ba1	Te1^{3}	72.12(17)
Te6^{5}	Ba1	Te1^{2}	69.14(4)
Te6^{5}	Ba1	Te2	121.75(17)
Te6^{5}	Ba1	Te4	140.90(7)
Te6^{5}	Ba1	Te6^{6}	4.6(4)
Ba1^{7}	Ba2	Ba1^{8}	109.51(3)
Te1	Ba2	Ba1^{7}	164.45(3)
Te1	Ba2	Ba1^{8}	55.926(18)
Te1^{9}	Ba2	Ba1^{7}	55.926(18)
Te1^{9}	Ba2	Ba1^{8}	164.45(3)
Te1	Ba2	Te1^{9}	137.76(4)
Te1^{9}	Ba2	Te2^{7}	110.62(2)
Te1	Ba2	Te2^{7}	110.62(2)
Te2	Ba2	Ba1^{7}	111.729(19)
Te2	Ba2	Ba1^{8}	111.729(19)
Te2^{7}	Ba2	Ba1^{8}	54.780(13)
Te2^{7}	Ba2	Ba1^{7}	54.780(13)
Te2^{10}	Ba2	Ba1^{7}	119.699(15)
Te2^{10}	Ba2	Ba1^{8}	119.699(15)
Te2^{10}	Ba2	Te1^{9}	75.26(2)
Te2	Ba2	Te1^{9}	73.02(2)
Te2	Ba2	Te1	73.02(2)
Te2^{10}	Ba2	Te1	75.26(2)
Te2^{10}	Ba2	Te2	80.94(5)
Te2^{10}	Ba2	Te2^{7}	147.08(5)
Te2	Ba2	Te2^{7}	131.97(5)
Te2^{10}	Ba2	Te4	142.34(4)
Te2	Ba2	Te4	69.66(3)
Te2^{10}	Ba2	Te4^{7}	142.34(4)
Te2	Ba2	Te4^{7}	69.66(3)
Te2	Ba2	Te5^{11}	140.77(3)
Te2	Ba2	Te5	140.77(3)
Te2^{10}	Ba2	Te5^{11}	78.57(3)
Te2^{10}	Ba2	Te5	78.57(3)
Te4^{7}	Ba2	Ba1^{8}	93.43(2)
Te4	Ba2	Ba1^{7}	93.43(2)
Te4	Ba2	Ba1^{8}	55.86(2)
Te4^{7}	Ba2	Ba1^{7}	55.86(2)
Te4^{7}	Ba2	Te1	115.73(4)
Te4^{7}	Te4	Ba2	67.653(19)
Te4^{7}	Te4	Ba2^{7}	67.653(19)
Te4^{7}	Te4	Ba2^{2}	67.652(19)
Ba1^{10}	Te5	Ba1^{14}	103.73(3)
Ba1^{10}	Te5	Ba1^{8}	103.72(3)
Ba1^{8}	Te5	Ba1^{14}	103.73(3)
Ba2^{15}	Te5	Ba1^{8}	91.335(17)
Ba2^{15}	Te5	Ba1^{14}	72.12(3)
Ba2^{11}	Te5	Ba1^{8}	164.94(3)
Ba2	Te5	Ba1^{10}	91.334(17)
Ba2	Te5	Ba1^{8}	72.12(3)
Ba2^{11}	Te5	Ba1^{10}	72.12(3)
Ba2^{11}	Te5	Ba1^{14}	91.334(17)
Ba2^{15}	Te5	Ba1^{10}	164.94(3)
Ba2	Te5	Ba1^{14}	164.94(3)
Ba2	Te5	Ba2^{11}	93.29(3)
Ba2^{11}	Te5	Ba2^{15}	93.29(3)
Ba2	Te5	Ba2^{15}	93.29(3)
Te6	Te5	Ba1^{8}	65.26(3)
Te6	Te5	Ba1^{10}	65.26(3)
Te6	Te5	Ba1^{14}	65.26(3)
Te6	Te5	Ba2^{15}	122.90(2)
Te6	Te5	Ba2	122.90(2)
Te6	Te5	Ba2^{11}	122.90(2)
Ba1^{14}	Te6	Ba1^{16}	69.25(4)
Ba1^{10}	Te6	Ba1^{3}	92.23(3)
Ba1^{8}	Te6	Ba1^{3}	69.25(4)
Ba1^{10}	Te6	Ba1^{17}	69.25(4)
Ba1^{3}	Te6	Ba1^{17}	97.0(2)
Ba1^{8}	Te6	Ba1^{16}	92.23(3)
Ba1^{10}	Te6	Ba1^{16}	164.37(11)
Ba1^{14}	Te6	Ba1^{3}	164.37(11)
Ba1^{8}	Te6	Ba1^{17}	164.37(11)
Ba1^{10}	Te6	Ba1^{14}	102.8(2)
Ba1^{10}	Te6	Ba1^{8}	102.8(2)
Ba1^{17}	Te6	Ba1^{16}	97.0(2)
Ba1^{3}	Te6	Ba1^{16}	97.0(2)
Ba1^{14}	Te6	Ba1^{17}	92.23(3)
Ba1^{8}	Te6	Ba1^{14}	102.8(2)
Te5	Te6	Ba1^{16}	120.11(17)

Te4	Ba2	Te1[9]	115.73(4)	Te5	Te6	Ba1[3]	120.11(17)
Te4[7]	Ba2	Te1[9]	74.02(3)	Te5	Te6	Ba1[17]	120.11(17)
Te4	Ba2	Te1	74.02(3)	Te5	Te6	Ba1[8]	64.51(19)
Te4	Ba2	Te2[7]	66.12(3)	Te5	Te6	Ba1[14]	64.51(19)
Te4[7]	Ba2	Te2[7]	66.12(3)	Te5	Te6	Ba1[10]	64.51(19)
Te4	Ba2	Te4[7]	44.69(4)	Te1[18]	Sn1	Te1[19]	91.66(2)
Te5	Ba2	Ba1[8]	54.06(2)	Te1[18]	Sn1	Te1[10]	87.70(4)
Te5[11]	Ba2	Ba1[7]	54.06(2)	Te1[18]	Sn1	Te1[4]	88.99(4)
Te5[11]	Ba2	Ba1[8]	107.47(3)	Te1[4]	Sn1	Te1	91.66(2)
Te5	Ba2	Ba1[7]	107.48(3)	Te1[19]	Sn1	Te1[10]	88.99(4)
Te5	Ba2	Te1[9]	131.64(4)	Te1[3]	Sn1	Te1	88.99(4)
Te5[11]	Ba2	Te1[9]	69.58(3)	Te1[4]	Sn1	Te1[3]	87.70(4)
Te5	Ba2	Te1	69.58(3)	Te1[19]	Sn1	Te1	87.70(4)
Te5[11]	Ba2	Te1	131.64(4)	Te1[19]	Sn1	Te1[4]	179.10(5)
Te5[11]	Ba2	Te2[7]	73.92(3)	Te1[10]	Sn1	Te1	91.66(2)
Te5	Ba2	Te2[7]	73.92(3)	Te1[18]	Sn1	Te1[3]	91.66(2)
Te5	Ba2	Te4	109.91(3)	Te1[4]	Sn1	Te1[10]	91.66(2)
Te5	Ba2	Te4[7]	138.90(3)	Te1[3]	Sn1	Te1[10]	179.10(5)
Te5[11]	Ba2	Te4[7]	109.91(3)	Te1[18]	Sn1	Te1	179.10(5)
Te5[11]	Ba2	Te4	138.90(3)	Te1[19]	Sn1	Te1[3]	91.66(2)
Te5	Ba2	Te5[11]	65.80(5)	Te1	Sn2	Te1[10]	92.25(5)
Ba1	Te1	Ba1[8]	97.25(5)	Te1	Sn2	Te1[4]	92.25(5)
Ba1[10]	Te1	Ba1[3]	95.71(4)	Te1[10]	Sn2	Te1[4]	92.25(5)
Ba1	Te1	Ba1[3]	91.35(4)	Te1[10]	Sn2	Te2[10]	86.88(4)
Ba1[3]	Te1	Ba1[8]	68.63(2)	Te1[10]	Sn2	Te2	178.30(5)
Ba1	Te1	Ba1[10]	159.55(3)	Te1	Sn2	Te2[12]	178.30(5)
Ba1[10]	Te1	Ba1[8]	103.20(5)	Te1[4]	Sn2	Te2	89.24(3)
Ba1	Te1	Ba2	96.01(4)	Te1	Sn2	Te2	86.88(4)
Ba1[10]	Te1	Ba2	91.57(4)	Te1[10]	Sn2	Te2[12]	89.24(3)
Ba2	Te1	Ba1[8]	69.30(3)	Te1[4]	Sn2	Te2[12]	86.88(4)
Ba2	Te1	Ba1[3]	137.87(3)	Te1	Sn2	Te2[10]	89.24(3)
Sn1	Te1	Ba1[10]	80.90(3)	Te1[4]	Sn2	Te2[10]	178.30(5)
Sn1	Te1	Ba1[8]	145.71(3)	Te2[12]	Sn2	Te2	91.65(5)
Sn1	Te1	Ba1[3]	77.11(2)	Te2[10]	Sn2	Te2	91.65(5)
Sn1	Te1	Ba1	82.02(3)	Te2[10]	Sn2	Te2[12]	91.65(5)
Sn1	Te1	Ba2	144.98(3)				

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

Table SV. Crystallographic parameters of $Ba_9Sn_3(Te_{0.8}Se_{0.2})_{15}$.

Crystallographic data of $Ba_9Sn_3(Te_{0.8}Se_{0.2})_{15}$					
Formula : $Ba_9Sn_3(Te_{0.8}Se_{0.2})_{15}$		Z = 2			
Crystal system : hexagonal		Calculated unit cell formula weight: 6712.25(0) g/mol			
Space group : P -6c2 (188)					
Crystal parameters: *a* = *b* = 10.1850(2) (Å); *c* = 20.4055(7) (Å); V = 1833.17(0) (Å^3)					
χ^2 = 6.0(1); Rp = 3.2(5)% Rwp = 5.0(3)%					
Atamic parameters					
Atom	wyck.	x	y	z	Occ.
Ba1	12l	-0.0041(8)	0.3712 (9)	0.0856(0)	1
Ba2	6k	0.3763(5)	0.3804 (1)	0.2500(0)	1
Sn1	2a	0.0000(0)	0.0000(0)	0.0000(0)	0.973(2)
Sn2	4g	0.0000(0)	0.0000(0)	0.1654(8)	0.976(7)
Te1	12l	0.2578(7)	0.2483 (9)	0.0836 (6)	0.567(3)
Se1	12l	0.2419(0)	0.2492(7)	0.0872(2)	0.432(7)
Te2	6k	-0.0042(4)	0.2505(3)	0.2500(0)	0.932(7)
Se2	6k	-0.0035(9)	0.2702(7)	0.2500(0)	0.035(9)
Te3	2c	0.3333(3)	0.6666(7)	0.0000(0)	1
Se3	2c	0.3333(3)	0.6666(7)	0.0000(0)	0
Te4	4h	0.3333(3)	0.6666(7)	0.1704(5)	1
Se4	4h	0.3333(3)	0.6666(7)	0.1622(2)	0
Te5	4i	0.6666(7)	0.3333(3)	0.1704(2)	1
Se5	4i	0.6666(7)	0.3333(3)	0.1742(0)	0
Te6	4i	0.6666(7)	0.3333(3)	0.1251(7)	0.5
Se6	4i	0.6666(7)	0.3333(3)	0.2604(9)	0

Table SVI. Crystallographic parameters of $Ba_9Sn_3(Te_{0.6}Se_{0.4})_{15}$.

Crystallographic data of $Ba_9Sn_3(Te_{0.6}Se_{0.4})_{15}$

Formula : $Ba_9Sn_3(Te_{0.6}Se_{0.4})_{15}$ Z = 2

Crystal system : hexagonal Calculated unit cell formula weight: 6122.32(0) g/mol

Space group : P -6c2 (188)

Crystal parameters: $a = b = 10.1209(0)$ (Å); $c = 20.0549(3)$ (Å); V = 1779.05(7) ($Å^3$)

$\chi^2 = 2.8(4)$; Rp = 3.2(0)% Rwp = 4.4(6)%

Atamic parameters

Atom	wyck.	x	y	z	Occ.
Ba1	12l	-0.0014(2)	0.3714 (3)	0.0850(8)	1
Ba2	6k	0.3679(6)	0.3677 (6)	0.2500(0)	1
Sn1	2a	0.0000(0)	0.0000(0)	0.0000(0)	0.815(9)
Sn2	4g	0.0000(0)	0.0000(0)	0.1758(4)	0.853(8)
Te1	12l	0.2431(5)	0.2229(0)	0.0866(7)	0.335(2)
Se1	12l	0.2478(0)	0.2469(4)	0.0860(9)	0.664(8)
Te2	6k	-0.0258(0)	0.2501(3)	0.2500(0)	0.348(1)
Se2	6k	-0.0025(5)	0.2646(5)	0.2500(0)	0.651(9)
Te3	2c	0.3333(3)	0.6666(7)	0.0000(0)	1
Se3	2c	0.3333(3)	0.6666(7)	0.0000(0)	0
Te4	4h	0.3333(3)	0.6666(7)	0.1609(2)	0.774(9)
Se4	4h	0.3333(3)	0.6666(7)	0.1673(4)	0.225(1)
Te5	4i	0.6666(7)	0.3333(3)	0.1557(8)	0.861(3)
Se5	4i	0.6666(7)	0.3333(3)	0.1617(2)	0.138(7)
Te6	4i	0.6666(7)	0.3333(3)	0.0006 (6)	0.5
Se6	4i	0.6666(7)	0.3333(3)	0.0006(6)	0

Table SVII. Crystallographic parameters of $Ba_9Sn_3(Te_{0.4}Se_{0.6})_{15}$.

Crystallographic data of $Ba_9Sn_3(Te_{0.4}Se_{0.6})_{15}$					
Formula : $Ba_9Sn_3(Te_{0.4}Se_{0.6})_{15}$		Z = 2			
Crystal system : hexagonal		Calculated unit cell formula weight: 5908.11(6)g/mol			
Space group : P -6c2 (188)					
Crystal parameters: $a = b$ = 9.9850(3) (Å); c = 19.8115 (4) (Å); V = 1710.52(1) ($Å^3$)					
χ^2 = 5.1(2); Rp = 2.8(6)% Rwp = 4.3(5)%					
Atamic parameters					
Atom	wyck.	x	y	z	Occ.
Ba1	12l	0.0011(3)	0.3743 (1)	0.0845(1)	1
Ba2	6k	0.3721(7)	0.3631(4)	0.2500(0)	1
Sn1	2a	0.0000(0)	0.0000(0)	0.0000(0)	0.875(1)
Sn2	4g	0.0000(0)	0.0000(0)	0.1741(0)	0.792(4)
Te1	12l	0.2389(7)	0.2568(5)	0.0843(4)	0.222(5)
Se1	12l	0.2300(2)	0.2396(3)	0.0852(3)	0.777(5)
Te2	6k	0.0222(2)	0.2817(2)	0.2500(0)	0
Se2	6k	0.0232(0)	0.2935(3)	0.2500(0)	1
Te3	2c	0.3333(3)	0.6666(7)	0.0000(0)	1
Se3	2c	0.3333(3)	0.6666(7)	0.0000(0)	0
Te4	4h	0.3333(3)	0.6666(7)	0.1738(5)	0.395(9)
Se4	4h	0.3333(3)	0.6666(7)	0.1667(7)	0.604(1)
Te5	4i	0.6666(7)	0.3333(3)	0.1538(4)	0.941(1)
Se5	4i	0.6666(7)	0.3333(3)	0.1538(4)	0.142(8)
Te6	4i	0.6666(7)	0.3333(3)	0.0006 (6)	0.5
Se6	4i	0.6666(7)	0.3333(3)	0.0006(6)	0

Table SVIII. Crystallographic parameters of $Ba_9Sn_3(Te_{0.2}Se_{0.8})_{15}$.

Crystallographic data of $Ba_9Sn_3(Te_{0.2}Se_{0.8})_{15}$					
Formula : $Ba_9Sn_3(Te_{0.2}Se_{0.8})_{15}$		Z = 2			
Crystal system : hexagonal		Calculated unit cell formula weight: 5656.63(3)g/mol			
Space group : P -6c2 (188)					
Crystal parameters: $a = b$ = 9.7846(3) (Å); c = 19.7379(0) (Å); V = 1636.51(7) ($Å^3$)					
χ^2 = 5.7(1); Rp = 3.0(8)% Rwp = 4.7(3)%					
Atamic parameters					
Atom	wyck.	x	y	z	Occ.
Ba1	12l	-0.0159(1)	0.3757 (4)	0.0863(7)	1
Ba2	6k	0.3611(9)	0.3796(1)	0.2500(0)	1
Sn1	2a	0.0000(0)	0.0000(0)	0.0000(0)	0.638(6)
Sn2	4g	0.0000(0)	0.0000(0)	0.1781(6)	0.761(0)
Te1	12l	0.2406(1)	0.2040(5)	0.0773(7)	0.048(8)
Se1	12l	0.2351(1)	0.2317 (7)	0.0789 (4)	0.955(7)
Te2	6k	-0.0248(6)	0.2651(5)	0.2500(0)	0
Se2	6k	-0.0170(1)	0.2596(0)	0.2500(0)	1
Te3	2c	0.3333(3)	0.6666(7)	0.0000(0)	0
Se3	2c	0.3333(3)	0.6666(7)	0.0000(0)	1
Te4	4h	0.3333(3)	0.6666(7)	0.1537(7)	0.390(2)
Se4	4h	0.3333(3)	0.6666(7)	0.1562(4)	0.612(0)
Te5	4i	0.6666(7)	0.3333(3)	0.1816(3)	0.965(7)
Se5	4i	0.6666(7)	0.3333(3)	0.1869(5)	0.037(3)
Te6	4i	0.6666(7)	0.3333(3)	0.0062 (9)	0
Se6	4i	0.6666(7)	0.3333(3)	0.0170(6)	0.5

Table SIX. Crystallographic parameters of $Ba_9Sn_3Se_{15}$.

Crystallographic data of $Ba_9Sn_3Se_{15}$					
Formula : $Ba_9Sn_3Se_{15}$		Z = 2			
Crystal system : hexagonal		Calculated unit cell formula weight: 5334.07(9) g/mol			
Space group : P -6c2 (188)					
Crystal parameters: $a = b = 9.7209(3)$ (Å); $c = 19.5817(1)$ (Å); V = 1602.489(1) ($Å^3$)					
$\chi^2 = 2.9(1)$; Rp = 3.4(0)% Rwp = 4.6(2)%					
Atamic parameters					
Atom	wyck.	x	y	z	Occ.
Ba1	12l	0.0040(8)	0.3746(9)	0.0833(3)	1
Ba2	6k	0.3765(3)	0.3772(0)	0.2500(0)	1
Sn1	2a	0.0000(0)	0.0000(0)	0.0000(0)	0.713(1)
Sn2	4g	0.0000(0)	0.0000(0)	0.1478(9)	0.662(2)
Se1	12l	0.2638(9)	0.2656(6)	0.0828(4)	1
Se2	6k	0.0041(3)	0.2309(1)	0.2500(0)	1
Se3	2c	0.3333(3)	0.6666(7)	0.0000(0)	1
Se4	4h	0.3333(3)	0.6666(7)	0.1710(2)	1
Se5	4i	0.6666(7)	0.3333(3)	0.1553(6)	1
Se6	4i	0.6666(7)	0.3333(3)	0.0270(2)	0.5

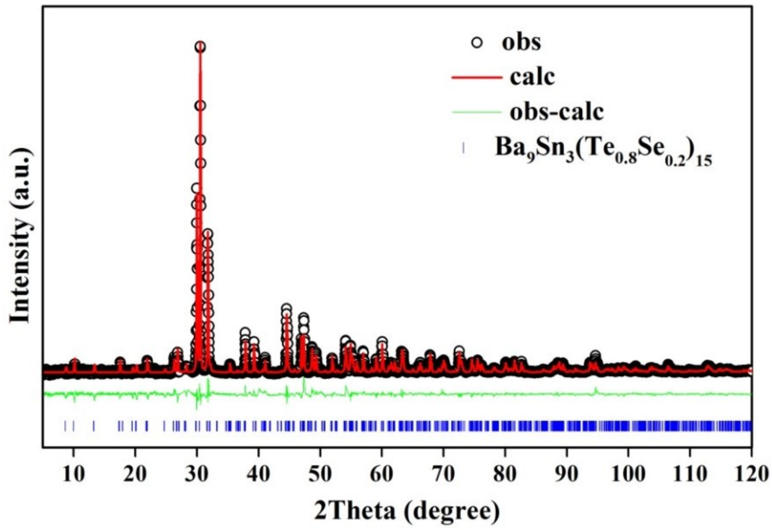

Fig.S1 The power X-ray diffraction and its refinement for $Ba_9Sn_3(Te_{0.8}Se_{0.2})_{15}$.

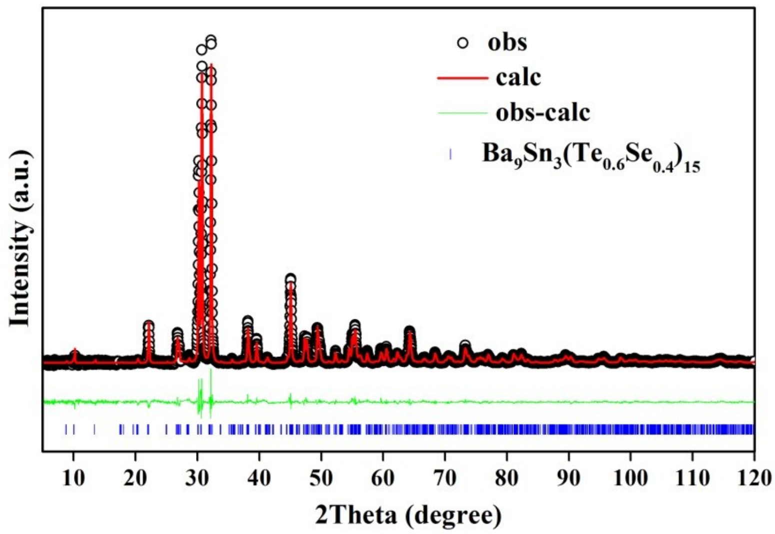

Fig.S2 The power X-ray diffraction and its refinement for $Ba_9Sn_3(Te_{0.6}Se_{0.4})_{15}$.

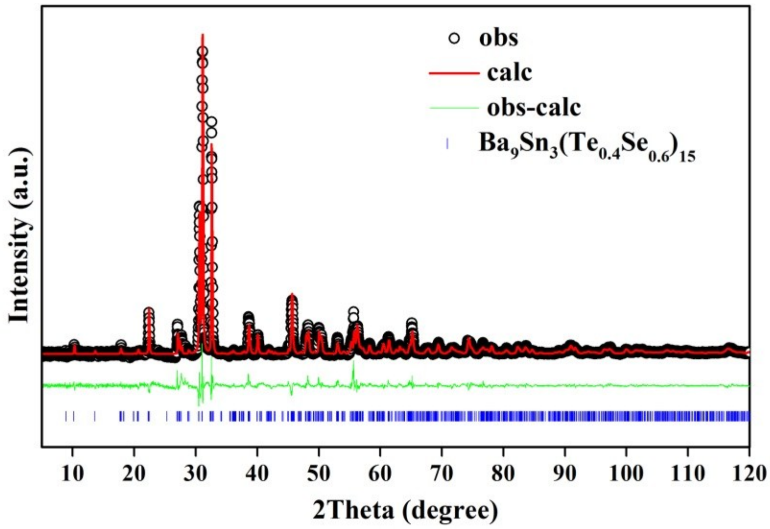

Fig.S3 The power X-ray diffraction and its refinement for $Ba_9Sn_3(Te_{0.4}Se_{0.6})_{15}$.

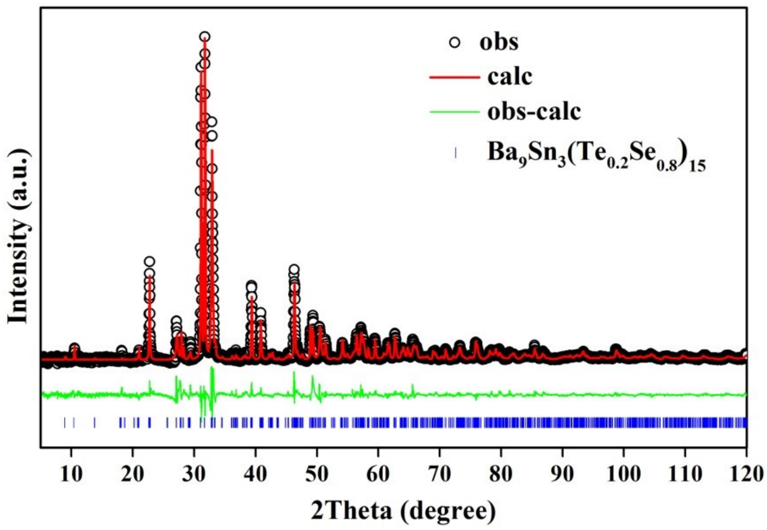

Fig.S4 The power X-ray diffraction and its refinement for $Ba_9Sn_3(Te_{0.2}Se_{0.8})_{15}$.

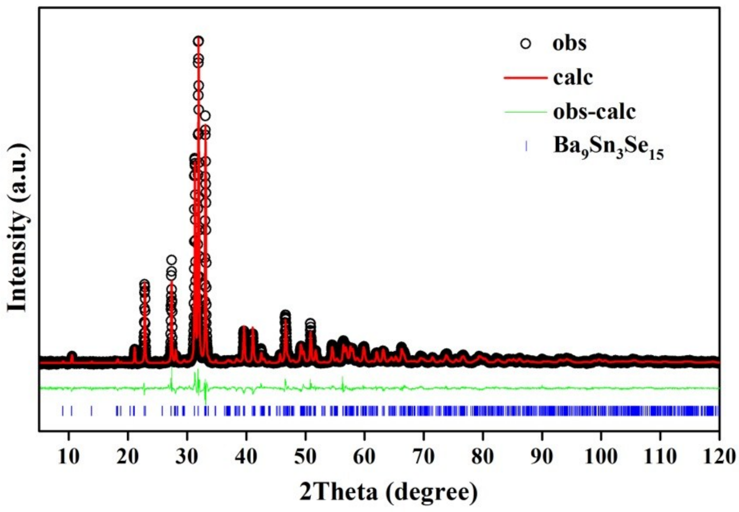

Fig.S5 The power X-ray diffraction and its refinement for $Ba_9Sn_3Se_{15}$.