Crystal Structure, Phase Width, and Physical Properties of the Barium Tetrel Selenides $Ba_6Si_{2-x}Ge_xSe_{12}$ (x = 0, 0.5, 1, and 1.5) with Ultralow Thermal Conductivity

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SUPPORTING INFORMATION

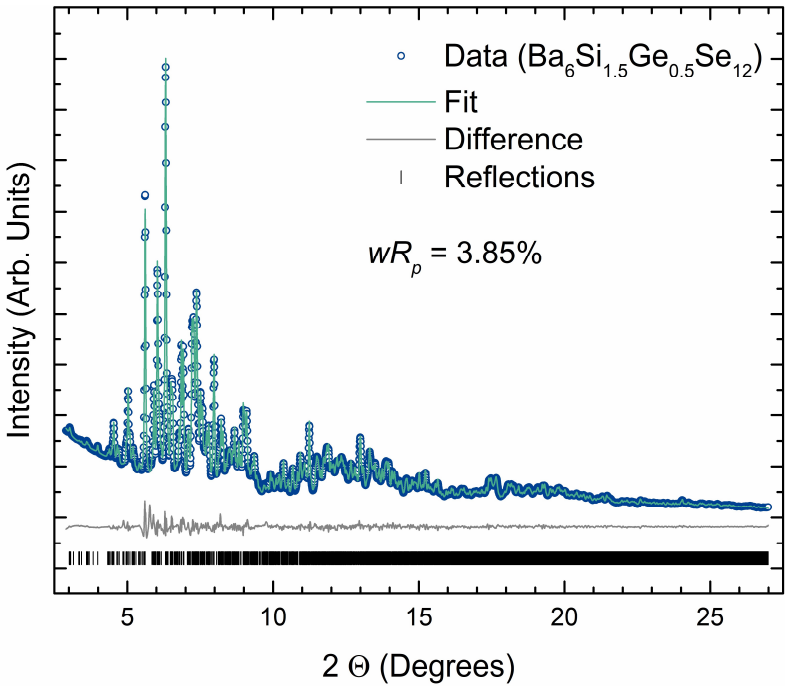

Fig. S1 Rietveld refinement plot for $Ba_6Si_{2-x}Ge_xSe_{12}$ for x = 0.5 including the Se4 and Se14 sites.

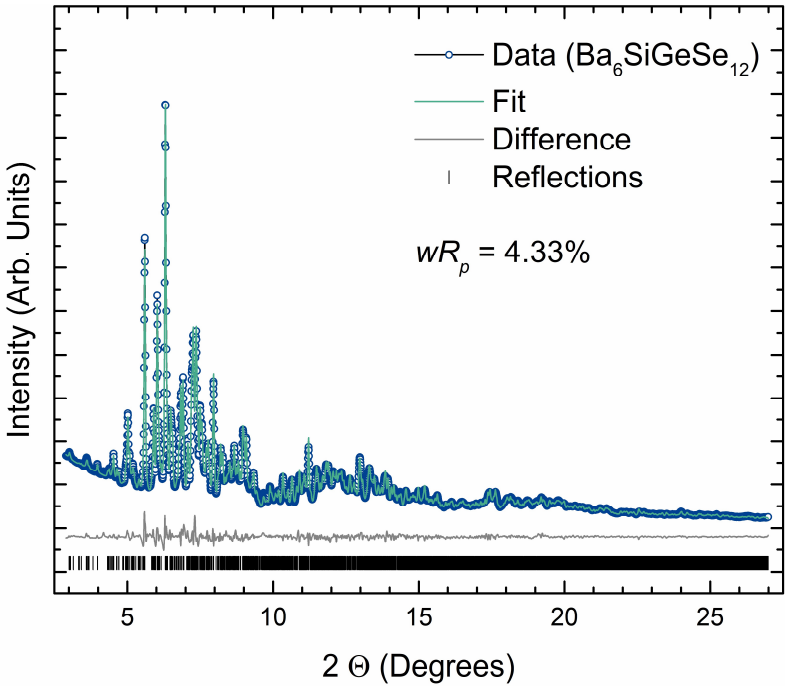

Fig. S2 Rietveld refinement plot for $Ba_6Si_{2-x}Ge_xSe_{12}$ for x = 1 including the Se4 and Se14 sites.

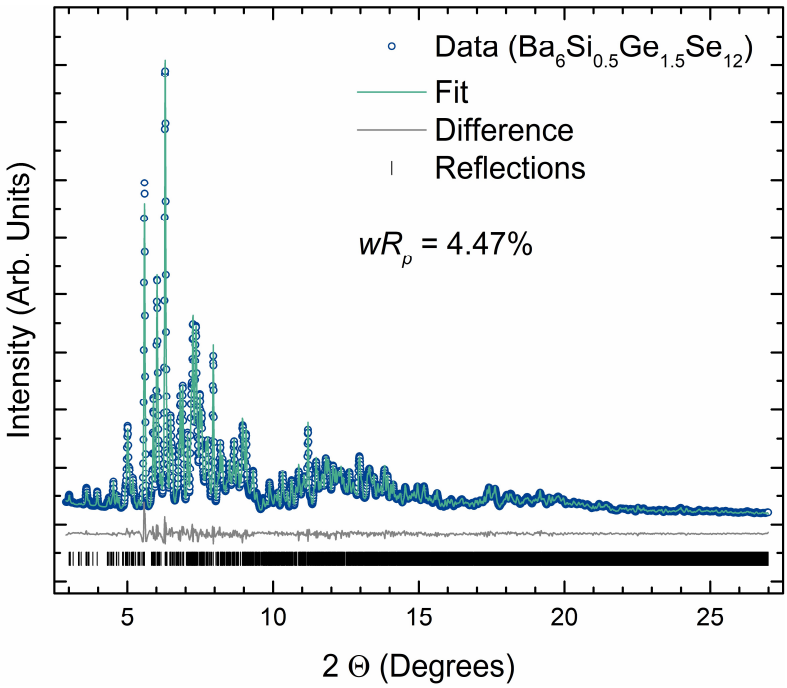

Fig. S3 Rietveld refinement plot for $Ba_6Si_{2-x}Ge_xSe_{12}$ for x = 1.5 including the Se4 and Se14 sites.

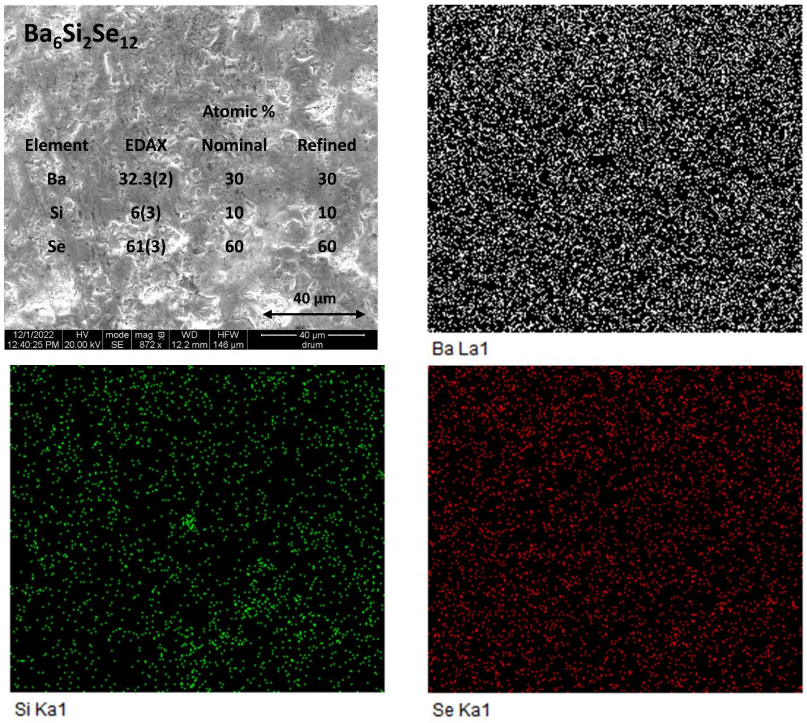

Fig. S4 EDAX and elemental mapping of the hot-pressed $Ba_6Si_2Se_{12}$ pellet.

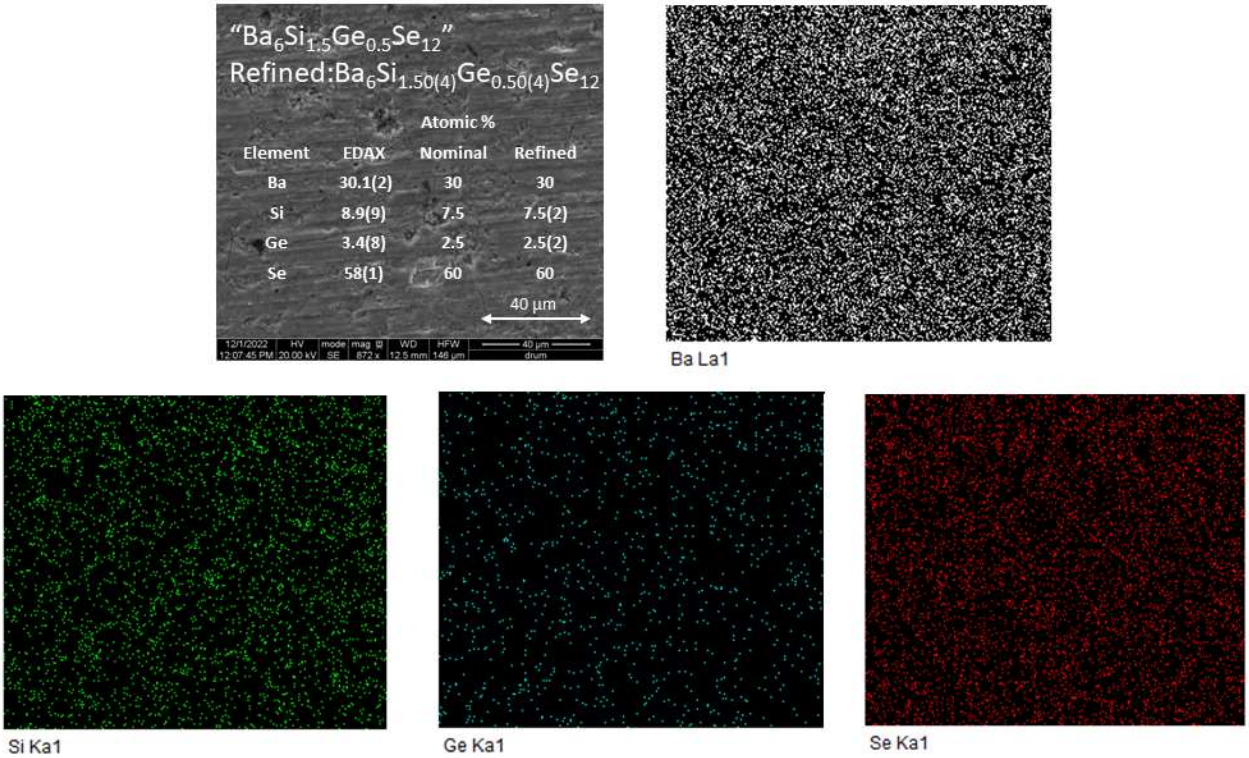

Fig. S5 EDAX and elemental mapping of the hot-pressed $Ba_6Si_{1.5}Ge_{0.5}Se_{12}$ pellet.

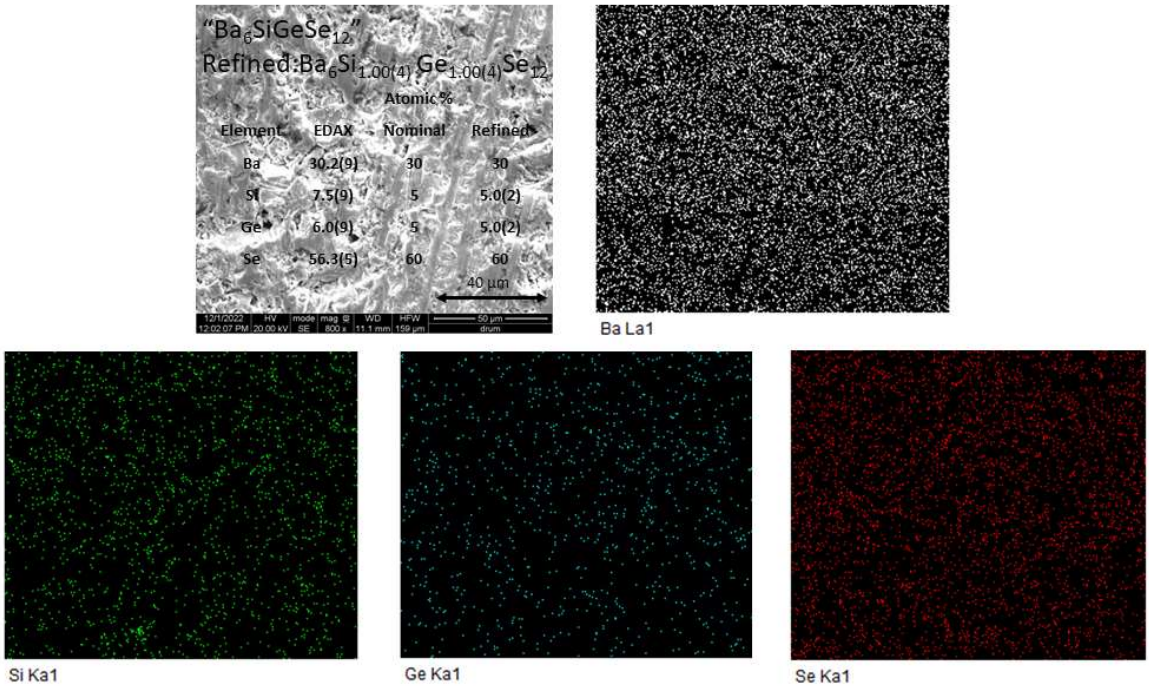

Fig. S6 EDAX and elemental mapping of the hot-pressed $Ba_6SiGeSe_{12}$ pellet.

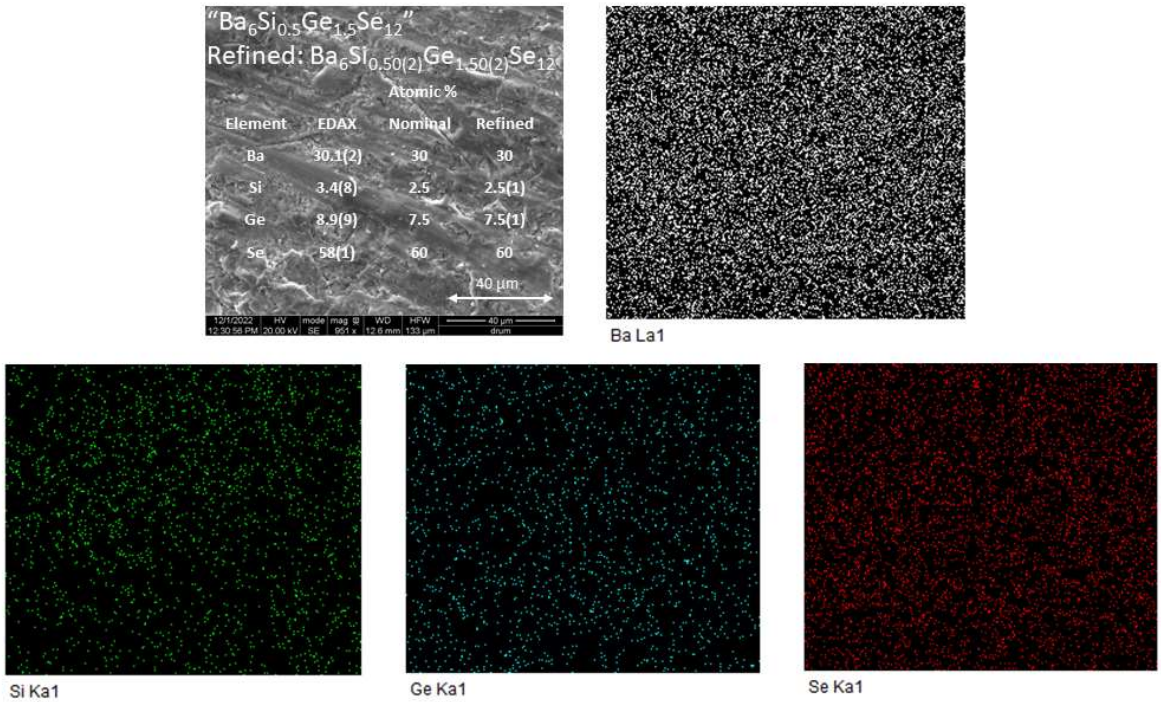

Fig. S7 EDAX and elemental mapping of the hot-pressed $Ba_6Si_{0.5}Ge_{1.5}Se_{12}$ pellet.

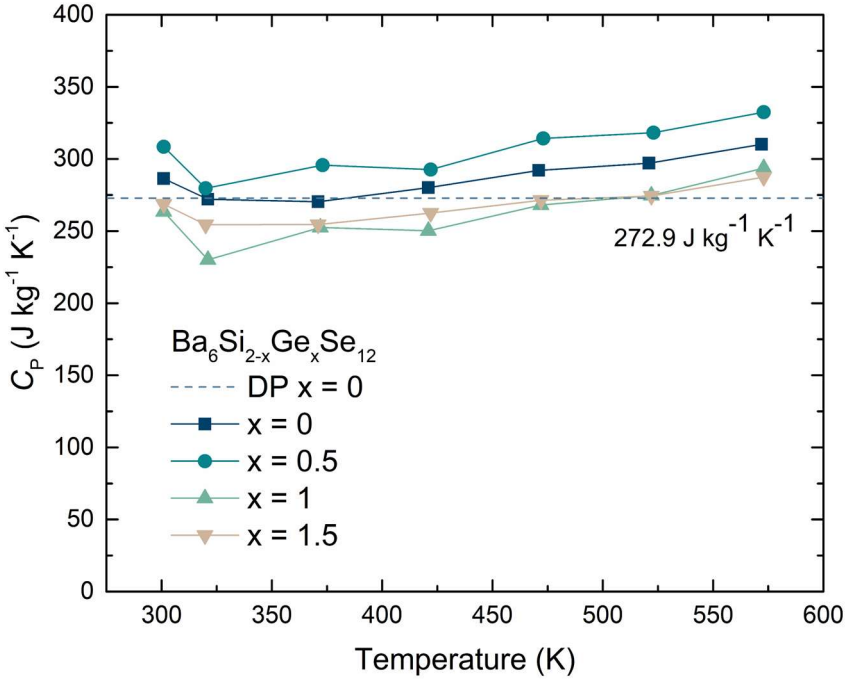

Fig. S8 Specific heat capacity curves of the $Ba_6Si_{2-x}Ge_xSe_{12}$ samples and the Dulong-Petit limit of $Ba_6Si_2Se_{12}$.

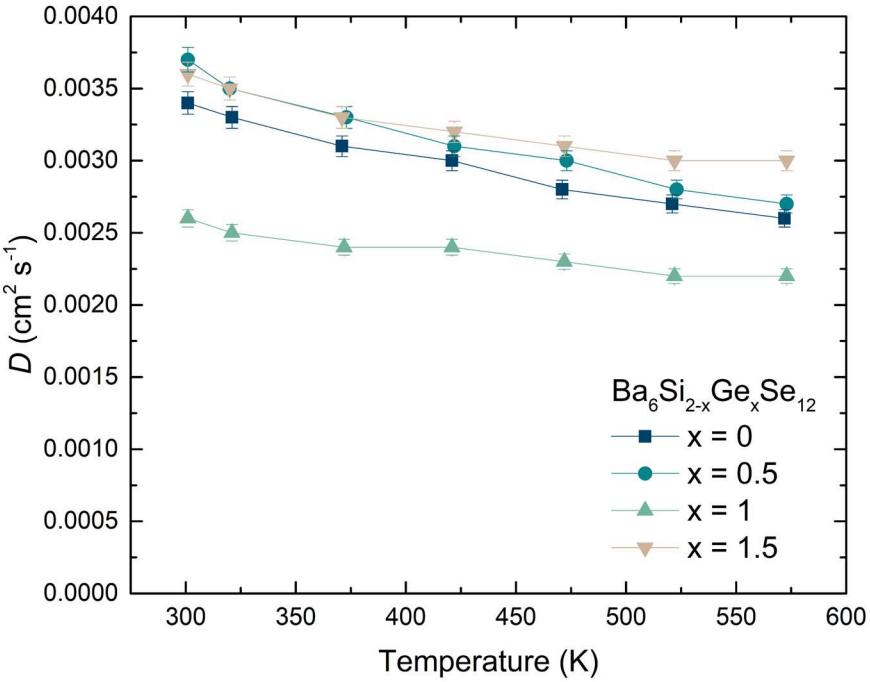

Fig. S9 Thermal diffusivity curves of the $Ba_6Si_{2-x}Ge_xSe_{12}$ samples.

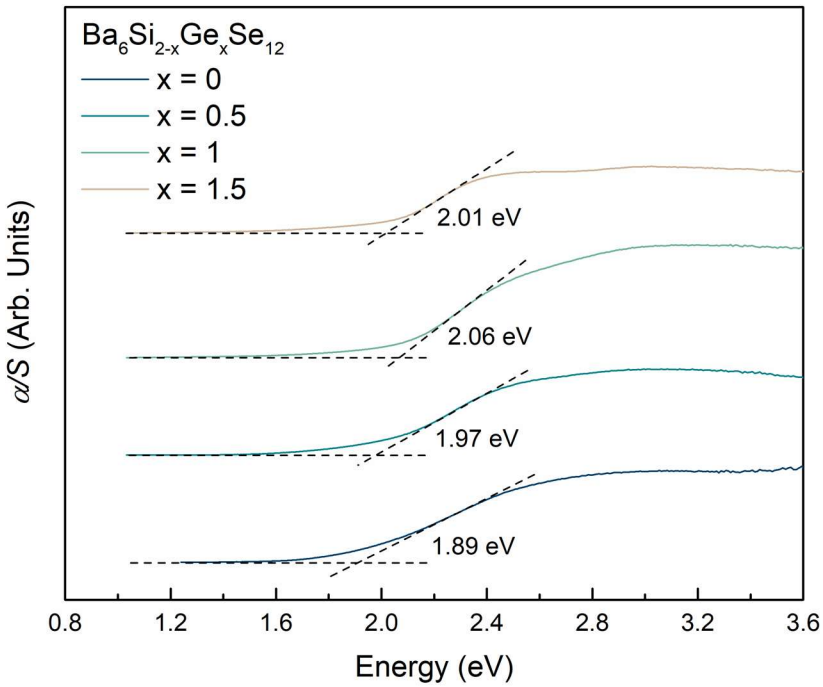

Fig. S10 Absorption spectra and band gap determination of the $Ba_6Si_{2-x}Ge_xSe_{12}$ samples.

Table S1 Initial single crystal XRD model of $Ba_6Si_2Se_{12}$ with refined atomic positions, U_{eq}, and occupancies. a = 9.1830(12) Å, b = 12.2668(16) Å, c = 12.3522(17) Å, α = 109.281(3)º, β = 104.699(3)º, γ = 100.447(3)º, R_1 = 0.0574, wR_2 = 0.1751, GOF = 1.175.

Atom	Site	x	y	z	U_{eq} / Å^2	occ.
Ba1	2*i*	0.07713(13)	0.36082(10)	0.60275(10)	0.0181(2)	1
Ba2	2*i*	0.09028(13)	0.93737(10)	0.17663(10)	0.0178(2)	1
Ba3	2*i*	0.28767(15)	0.57805(11)	0.06064(12)	0.0243(3)	1
Ba4	2*i*	0.31556(14)	0.36150(11)	0.30239(12)	0.0225(2)	1
Ba5	2*i*	0.34148(13)	0.07302(10)	0.59649(10)	0.0170(2)	1
Ba6	2*i*	0.65126(13)	0.16125(10)	0.17112(10)	0.0184(2)	1
Si1	2*i*	0.6109(5)	0.2779(4)	0.5281(4)	0.0115(8)	1
Si2	2*i*	0.6362(5)	0.7803(4)	0.0424(4)	0.0123(8)	1
Se1	2*i*	0.0095(2)	0.20011(18)	0.31176(18)	0.0193(4)	1
Se2	2*i*	0.0112(2)	0.07529(18)	0.42429(18)	0.0202(4)	1
Se3	2*i*	0.0358(4)	0.3423(3)	0.0307(3)	0.0221(7)	0.644(6)
Se5	2*i*	0.0614(4)	0.6076(3)	0.8048(3)	0.0273(8)	0.644(6)
Se4	2*i*	0.0458(7)	0.4933(6)	0.1832(6)	0.0265(14)	0.356(6)
Se14	2*i*	0.9390(9)	0.2811(6)	0.0829(7)	0.0358(17)	0.356(6)
Se6	2*i*	0.2022(2)	0.2644(2)	0.82078(19)	0.0244(4)	1
Se7	2*i*	0.2334(2)	0.78729(19)	0.35038(19)	0.0219(4)	1
Se8	2*i*	0.2442(2)	0.08590(19)	0.02163(19)	0.0208(4)	1
Se9	2*i*	0.2623(2)	0.59510(17)	0.53851(18)	0.0191(4)	1
Se10	2*i*	0.4506(2)	0.11734(16)	0.35779(16)	0.0174(3)	1
Se11	2*i*	0.4618(2)	0.36302(17)	0.62892(19)	0.0219(4)	1
Se12	2*i*	0.4677(2)	0.86868(17)	0.12078(17)	0.0185(4)	1

Table S2 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6Si_2Se_{12}$ sample. a = 9.1821(7) Å, b = 12.2634(15) Å, c = 12.3636(18) Å, α = 109.278(3)º, β = 104.732(2)º, γ = 100.4061(16)º.

Atom	Site	x	y	z	U_{iso} / Å^2	occ.
Ba1	2*i*	0.0742(8)	0.3597(6)	0.6023(6)	0.0214(5)	1
Ba2	2*i*	0.0942(8)	0.9395(6)	0.1750(6)	0.0214(5)	1
Ba3	2*i*	0.2870(8)	0.5731(6)	0.0611(6)	0.0214(5)	1
Ba4	2*i*	0.3159(8)	0.3620(6)	0.3019(6)	0.0214(5)	1
Ba5	2*i*	0.3429(8)	0.0760(6)	0.5964(6)	0.0214(5)	1
Ba6	2*i*	0.6513(8)	0.1582(6)	0.1674(7)	0.0214(5)	1
Si1	2*i*	0.6138(20)	0.2807(16)	0.5265(16)	0.0115	1
Si2	2*i*	0.630(2)	0.7801(18)	0.0415(16)	0.0123	1
Se1	2*i*	0.0062(11)	0.2017(9)	0.3163(10)	0.0176(6)	1
Se2	2*i*	0.0039(11)	0.0703(11)	0.4197(10)	0.0176(6)	1
Se3	2*i*	0.0253(18)	0.3462(15)	0.0332(14)	0.023(3)	0.666(10)
Se5	2*i*	0.0760(19)	0.6071(16)	0.8090(14)	0.023(3)	0.666(10)
Se4	2*i*	0.001(4)	0.480(3)	0.165(3)	0.023(3)	0.334(10)
Se14	2*i*	0.946(4)	0.271(3)	0.083(3)	0.023(3)	0.334(10)
Se6	2*i*	0.2037(13)	0.2679(9)	0.8181(9)	0.0176(6)	1
Se7	2*i*	0.2241(12)	0.7849(9)	0.3482(9)	0.0176(6)	1
Se8	2*i*	0.2474(12)	0.0896(10)	0.0203(10)	0.0176(6)	1
Se9	2*i*	0.2662(12)	0.5945(10)	0.5446(9)	0.0176(6)	1
Se10	2*i*	0.4484(12)	0.1174(9)	0.3561(9)	0.0176(6)	1
Se11	2*i*	0.4645(12)	0.3611(10)	0.6314(10)	0.0176(6)	1
Se12	2*i*	0.4578(12)	0.8662(11)	0.1174(10)	0.0176(6)	1

Table S3 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6Si_{1.5}Ge_{0.5}Se_{12}$ sample. a = 9.1883(6) Å, b = 12.2785(13) Å, c = 12.3890(16) Å, α = 109.269(3)º, β = 104.737(2)º, γ = 100.4291(15)º.

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0764(7)	0.3609(5)	0.6008(5)	0.0179(4)	1
Ba2	2*i*	0.0939(7)	0.9385(5)	0.1758(5)	0.0179(4)	1
Ba3	2*i*	0.2867(7)	0.5760(5)	0.0575(5)	0.0179(4)	1
Ba4	2*i*	0.3160(7)	0.3609(5)	0.3025(6)	0.0179(4)	1
Ba5	2*i*	0.3432(7)	0.0747(5)	0.5973(5)	0.0179(4)	1
Ba6	2*i*	0.6541(7)	0.1604(5)	0.1708(6)	0.0179(4)	1
Si1	2*i*	0.6107(15)	0.2742(13)	0.5297(13)	0.0115	0.759(18)
Ge1	2*i*	0.6107(15)	0.2742(13)	0.5297(13)	0.0115	0.241(18)
Si2	2*i*	0.6350(16)	0.7813(14)	0.0371(13)	0.0123	0.741(18)
Ge2	2*i*	0.6350(16)	0.7813(14)	0.0371(13)	0.0123	0.259(18)
Se1	2*i*	0.0056(10)	0.1957(9)	0.3090(9)	0.0233(6)	1
Se2	2*i*	0.0066(10)	0.0719(10)	0.4208(9)	0.0233(6)	1
Se3	2*i*	0.0352(15)	0.3436(13)	0.0345(12)	0.0161(2)	0.650(8)
Se5	2*i*	0.0586(16)	0.6060(13)	0.8052(13)	0.0161(2)	0.650(8)
Se4	2*i*	0.042(3)	0.498(2)	0.187(2)	0.0161(2)	0.350(8)
Se14	2*i*	0.945(3)	0.288(2)	0.091(2)	0.0161(2)	0.350(8)
Se6	2*i*	0.2008(11)	0.2661(8)	0.8195(8)	0.0233(6)	1
Se7	2*i*	0.2350(11)	0.7894(8)	0.3518(8)	0.0233(6)	1
Se8	2*i*	0.2440(11)	0.0832(9)	0.0211(9)	0.0233(6)	1
Se9	2*i*	0.2592(11)	0.5912(9)	0.5350(8)	0.0233(6)	1
Se10	2*i*	0.4501(11)	0.1186(8)	0.3572(9)	0.0233(6)	1
Se11	2*i*	0.4607(11)	0.3619(9)	0.6304(9)	0.0233(6)	1
Se12	2*i*	0.4695(10)	0.8703(10)	0.1226(9)	0.0233(6)	1
Se13	2*i*	0.5147(12)	0.3896(9)	0.1223(10)	0.0233(6)	1

Table S4 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6SiGeSe_{12}$ sample. *a* = 9.1954(8) Å, *b* =12.2964(16) Å, *c* = 12.426(2) Å, α = 109.259(3)º, β = 104.774(3)º, γ = 100.4122(17)º.

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0763(8)	0.3579(6)	0.5978(6)	0.0196(5)	1
Ba2	2*i*	0.0968(8)	0.9407(5)	0.1749(6)	0.0196(5)	1
Ba3	2*i*	0.2797(8)	0.5749(6)	0.0568(6)	0.0196(5)	1
Ba4	2*i*	0.3180(8)	0.3616(6)	0.3000(7)	0.0196(5)	1
Ba5	2*i*	0.3415(8)	0.0740(6)	0.5952(6)	0.0196(5)	1
Ba6	2*i*	0.6534(8)	0.1605(6)	0.1683(7)	0.0196(5)	1
Si1	2*i*	0.6139(14)	0.2794(12)	0.5297(12)	0.0115	0.49(2)
Ge1	2*i*	0.6139(14)	0.2794(12)	0.5297(12)	0.0115	0.51(2)
Si2	2*i*	0.6342(15)	0.7804(13)	0.0418(12)	0.0123	0.51(2)
Ge2	2*i*	0.6342(15)	0.7804(13)	0.0418(12)	0.0123	0.49(2)
Se1	2*i*	0.0106(11)	0.1993(9)	0.3133(10)	0.0203(6)	1
Se2	2*i*	0.0014(11)	0.0683(11)	0.4189(10)	0.0203(6)	1
Se3	2*i*	0.0354(18)	0.3484(15)	0.0413(14)	0.013(3)	0.615(9)
Se5	2*i*	0.0694(19)	0.6115(15)	0.8053(14)	0.013(3)	0.615(9)
Se4	2*i*	0.026(3)	0.488(2)	0.181(2)	0.013(3)	0.385(9)
Se14	2*i*	0.968(3)	0.284(2)	0.087(2)	0.013(3)	0.385(9)
Se6	2*i*	0.2000(13)	0.2688(10)	0.8184(10)	0.0203(6)	1
Se7	2*i*	0.2231(12)	0.7841(9)	0.3490(10)	0.0203(6)	1
Se8	2*i*	0.2438(12)	0.0851(9)	0.0222(10)	0.0203(6)	1
Se9	2*i*	0.2659(13)	0.5883(10)	0.5409(9)	0.0203(6)	1
Se10	2*i*	0.4531(12)	0.1197(9)	0.3571(9)	0.0203(6)	1
Se11	2*i*	0.4573(12)	0.3642(9)	0.6333(10)	0.0203(6)	1
Se12	2*i*	0.4583(11)	0.8671(10)	0.1172(10)	0.0203(6)	1
Se13	2*i*	0.5168(13)	0.3936(10)	0.1209(10)	0.0203(6)	1

Table S5 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6Si_{0.5}Ge_{1.5}Se_{12}$ sample. a = 9.1986(5) Å, b = 12.3114(11) Å, c = 12.4532(14) Å, α = 109.250(2)º, β = 104.7701(19)º, γ = 100.4056(12)º.

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0779(6)	0.3600(4)	0.5985(4)	0.0177(3)	1
Ba2	2*i*	0.0945(6)	0.9395(4)	0.1766(5)	0.0177(3)	1
Ba3	2*i*	0.2802(6)	0.5755(4)	0.0557(5)	0.0177(3)	1
Ba4	2*i*	0.3173(6)	0.3621(4)	0.3015(5)	0.0177(3)	1
Ba5	2*i*	0.3443(6)	0.0739(4)	0.5965(5)	0.0177(3)	1
Ba6	2*i*	0.6532(6)	0.1596(4)	0.1678(5)	0.0177(3)	1
Si1	2*i*	0.6121(10)	0.2766(8)	0.5305(8)	0.0115	0.201(14)
Ge1	2*i*	0.6121(10)	0.2766(8)	0.5305(8)	0.0115	0.799(14)
Si2	2*i*	0.6372(11)	0.7803(9)	0.0428(9)	0.0123	0.299(14)
Ge2	2*i*	0.6372(11)	0.7803(9)	0.0428(9)	0.0123	0.701(14)
Se1	2*i*	0.0071(9)	0.2005(7)	0.3124(7)	0.0216(5)	1
Se2	2*i*	0.0062(8)	0.0715(8)	0.4207(8)	0.0216(5)	1
Se3	2*i*	0.0400(14)	0.3444(12)	0.0372(11)	0.017(2)	0.604(8)
Se5	2*i*	0.0588(15)	0.6087(12)	0.8036(12)	0.017(2)	0.604(8)
Se4	2*i*	0.032(2)	0.4929(16)	0.1827(18)	0.017(2)	0.396(8)
Se14	2*i*	0.958(2)	0.2926(17)	0.0827(17)	0.017(2)	0.396(8)
Se6	2*i*	0.1984(10)	0.2686(7)	0.8194(7)	0.0216(5)	1
Se7	2*i*	0.2262(9)	0.7889(7)	0.3515(7)	0.0216(5)	1
Se8	2*i*	0.2424(10)	0.0830(7)	0.0196(8)	0.0216(5)	1
Se9	2*i*	0.2610(9)	0.5895(8)	0.5390(7)	0.0216(5)	1
Se10	2*i*	0.4534(10)	0.1211(7)	0.3551(7)	0.0216(5)	1
Se11	2*i*	0.4588(10)	0.3640(7)	0.6368(8)	0.0216(5)	1
Se12	2*i*	0.4646(9)	0.8682(8)	0.1201(7)	0.0216(5)	1
Se13	2*i*	0.5153(10)	0.3951(7)	0.1209(8)	0.0216(5)	1

Table S6 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6Si_2Se_{12}$ sample without Se4 and Se14. a = 9.1802(7) Å, b = 12.2610(16) Å, c = 12.3604(20) Å, α = 109.275(3)º, β = 104.7356(26)º, γ = 100.4072(18)º.

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0732(9)	0.3608(7)	0.6002(7)	0.0185(5)	1
Ba2	2*i*	0.0933(9)	0.9384(6)	0.1735(6)	0.0185(5)	1
Ba3	2*i*	0.2863(8)	0.5734(6)	0.0628(7)	0.0185(5)	1
Ba4	2*i*	0.3176(9)	0.3588(7)	0.3009(7)	0.0185(5)	1
Ba5	2*i*	0.3404(8)	0.0759(7)	0.5941(7)	0.0185(5)	1
Ba6	2*i*	0.6542(9)	0.1567(7)	0.1691(7)	0.0185(5)	1
Si1	2*i*	0.604(3)	0.288(3)	0.535(3)	0.0115	1
Si2	2*i*	0.629(3)	0.758(3)	0.024(3)	0.0123	1
Se1	2*i*	0.0073(12)	0.2010(10)	0.3152(11)	0.0171(6)	1
Se2	2*i*	0.0008(12)	0.0637(11)	0.4153(11)	0.0171(6)	1
Se3	2*i*	0.0118(18)	0.3384(14)	0.0359(14)	**0.074(3)**	1
Se5	2*i*	0.0697(19)	0.6001(13)	0.8137(14)	**0.074(3)**	1
Se6	2*i*	0.2095(14)	0.2678(10)	0.8208(10)	0.0171(6)	1
Se7	2*i*	0.2179(13)	0.7864(10)	0.3484(10)	0.0171(6)	1
Se8	2*i*	0.2505(13)	0.0902(11)	0.0176(11)	0.0171(6)	1
Se9	2*i*	0.2606(13)	0.5984(10)	0.5477(10)	0.0171(6)	1
Se10	2*i*	0.4455(13)	0.1187(10)	0.3509(10)	0.0171(6)	1
Se11	2*i*	0.4605(14)	0.3634(11)	0.6305(11)	0.0171(6)	1
Se12	2*i*	0.4538(13)	0.8607(12)	0.1143(11)	0.0171(6)	1
Se13	2*i*	0.5109(15)	0.3871(11)	0.1189(12)	0.0171(6)	1

Table S7 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6Si_{1.5}Ge_{0.5}Se_{12}$ sample without Se4 and Se14. a = 9.1886(7) Å, b = 12.2786(15) Å, c = 12.3891(19) Å, α = 109.267(3)º, β = 104.7380(25)º, γ = 100.4316(17)º.

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0753(8)	0.3622(6)	0.6007(6)	0.0163(4)	1
Ba2	2*i*	0.0940(8)	0.9397(6)	0.1740(6)	0.0163(4)	1
Ba3	2*i*	0.2838(8)	0.5745(6)	0.0568(6)	0.0163(4)	1
Ba4	2*i*	0.3160(8)	0.3579(6)	0.2999(7)	0.0163(4)	1
Ba5	2*i*	0.3428(7)	0.0757(6)	0.5958(6)	0.0163(4)	1
Ba6	2*i*	0.6556(8)	0.1580(6)	0.1704(7)	0.0163(4)	1
Si1	2*i*	0.605(2)	0.262(2)	0.529(2)	0.0115	0.85(2)
Ge1	2*i*	0.605(2)	0.262(2)	0.529(2)	0.0115	0.15(2)
Si2	2*i*	0.6349(19)	0.7769(17)	0.0301(17)	0.0123	0.65(2)
Ge2	2*i*	0.6349(19)	0.7769(17)	0.0301(17)	0.0123	0.35(2)
Se1	2*i*	0.0084(12)	0.1963(10)	0.3099(10)	0.0203(6)	1
Se2	2*i*	0.0024(11)	0.0667(11)	0.4189(10)	0.0203(6)	1
Se3	2*i*	0.0241(16)	0.3325(12)	0.0331(12)	**0.069(3)**	1
Se5	2*i*	0.0497(17)	0.6057(12)	0.8147(13)	**0.069(3)**	1
Se6	2*i*	0.2042(13)	0.2666(9)	0.8184(10)	0.0203(6)	1
Se7	2*i*	0.2299(12)	0.7922(9)	0.3537(10)	0.0203(6)	1
Se8	2*i*	0.2474(13)	0.0821(10)	0.0192(10)	0.0203(6)	1
Se9	2*i*	0.2572(12)	0.5929(10)	0.5385(10)	0.0203(6)	1
Se10	2*i*	0.4472(13)	0.1176(9)	0.3534(10)	0.0203(6)	1
Se11	2*i*	0.4610(13)	0.3621(10)	0.6300(11)	0.0203(6)	1
Se12	2*i*	0.4665(12)	0.8689(11)	0.1207(11)	0.0203(6)	1
Se13	2*i*	0.5193(14)	0.3929(11)	0.1243(11)	0.0203(6)	1

Table S8 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6SiGeSe_{12}$ sample without Se4 and Se14. a = 9.1950(9) Å, b = 12.2971(18) Å, c = 12.4263(23) Å, α = 109.257(4)º, β = 104.7701(31)º, γ = 100.4126(20)º.

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0729(9)	0.3599(7)	0.5966(6)	0.0169(5)	1
Ba2	2*i*	0.0955(9)	0.9406(6)	0.1740(7)	0.0169(5)	1
Ba3	2*i*	0.2783(8)	0.5734(6)	0.0556(7)	0.0169(5)	1
Ba4	2*i*	0.3179(9)	0.3583(7)	0.2966(8)	0.0169(5)	1
Ba5	2*i*	0.3397(8)	0.0738(7)	0.5928(7)	0.0169(5)	1
Ba6	2*i*	0.6547(9)	0.1583(7)	0.1688(7)	0.0169(5)	1
Si1	2*i*	0.6100(19)	0.2764(17)	0.5255(17)	0.0115	0.56(2)
Ge1	2*i*	0.6100(19)	0.2764(17)	0.5255(17)	0.0115	0.44(2)
Si2	2*i*	0.6339(17)	0.7715(16)	0.0407(15)	0.0123	0.44(2)
Ge2	2*i*	0.6339(17)	0.7715(16)	0.0407(15)	0.0123	0.56(2)
Se1	2*i*	0.0124(12)	0.1995(10)	0.3116(11)	0.0186(7)	1
Se2	2*i*	-0.0006(12)	0.0615(12)	0.4153(11)	0.0186(7)	1
Se3	2*i*	0.0234(18)	0.3365(14)	0.0417(15)	**0.075(3)**	1
Se5	2*i*	0.053(2)	0.6002(13)	0.8108(15)	**0.075(3)**	1
Se6	2*i*	0.2031(14)	0.2687(10)	0.8194(11)	0.0186(7)	1
Se7	2*i*	0.2178(13)	0.7903(10)	0.3532(11)	0.0186(7)	1
Se8	2*i*	0.2486(14)	0.0849(11)	0.0200(12)	0.0186(7)	1
Se9	2*i*	0.2585(13)	0.5899(11)	0.5432(11)	0.0186(7)	1
Se10	2*i*	0.4517(14)	0.1200(10)	0.3530(11)	0.0186(7)	1
Se11	2*i*	0.4542(14)	0.3657(11)	0.6313(12)	0.0186(7)	1
Se12	2*i*	0.4555(13)	0.8629(11)	0.1166(11)	0.0186(7)	1
Se13	2*i*	0.5199(15)	0.3948(11)	0.1237(12)	0.0186(7)	1

Table S9 Rietveld refined atomic positions, U_{iso}, and occupancies of the $Ba_6Si_{0.5}Ge_{1.5}Se_{12}$ sample without Se4 and Se14. a = 9.1985(7) Å, b = 12.3118(14) Å, c = 12.4533(17) Å, α = 109.2472(30)º, β = 104.7677(23)º, γ = 100.4070(15)º

Atom	Site	x	y	z	U_{iso} /A^2	occ.
Ba1	2*i*	0.0763(7)	0.3622(5)	0.5985(5)	0.0161(4)	1
Ba2	2*i*	0.0932(7)	0.9397(5)	0.1754(6)	0.0161(4)	1
Ba3	2*i*	0.2793(7)	0.5749(5)	0.0556(6)	0.0161(4)	1
Ba4	2*i*	0.3171(7)	0.3593(5)	0.2981(6)	0.0161(4)	1
Ba5	2*i*	0.3428(7)	0.0740(5)	0.5939(5)	0.0161(4)	1
Ba6	2*i*	0.6528(7)	0.1566(5)	0.1666(6)	0.0161(4)	1
Si1	2*i*	0.6092(12)	0.2700(11)	0.5259(11)	0.0115	0.261(16)
Ge1	2*i*	0.6092(12)	0.2700(11)	0.5259(11)	0.0115	0.739(16)
Si2	2*i*	0.6363(13)	0.7757(11)	0.0415(10)	0.0123	0.239(16)
Ge2	2*i*	0.6363(13)	0.7757(11)	0.0415(10)	0.0123	0.761(16)
Se1	2*i*	0.0087(10)	0.2008(8)	0.3120(9)	0.0186(6)	1
Se2	2*i*	0.0029(10)	0.0654(9)	0.4192(9)	0.0186(6)	1
Se3	2*i*	0.0215(15)	0.3316(11)	0.0404(12)	**0.082(3)**	1
Se5	2*i*	0.0448(16)	0.5998(11)	0.8120(12)	**0.082(3)**	1
Se6	2*i*	0.2006(12)	0.2682(8)	0.8198(9)	0.0186(6)	1
Se7	2*i*	0.2214(11)	0.7927(8)	0.3536(9)	0.0186(6)	1
Se8	2*i*	0.2480(11)	0.0819(9)	0.0197(9)	0.0186(6)	1
Se9	2*i*	0.2564(11)	0.5908(9)	0.5405(9)	0.0186(6)	1
Se10	2*i*	0.4493(12)	0.1208(8)	0.3507(8)	0.0186(6)	1
Se11	2*i*	0.4582(12)	0.3654(9)	0.6341(9)	0.0186(6)	1
Se12	2*i*	0.4610(11)	0.8650(9)	0.1206(9)	0.0186(6)	1
Se13	2*i*	0.5186(12)	0.3963(9)	0.1207(9)	0.0186(6)	1