Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information - Vacancy and anti-site disorder scattering in $AgBiSe_2$ thermoelectrics

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Table S1. Crystallographic data (atomic coordinates, occupancy, and U_{iso}) of $AgBiSe_2$, obtained from Rietveld refinements of X-ray synchrotron diffraction.

$AgBiSe_2$ structure from X-ray powder diffraction (space group $P\bar{3}m1$) a = 4.19231(8) Å; c = 19.6622(2) Å; 16.1 % $R\bar{3}m$ Fit residuals (R_{wp}, R_{exp}, χ^2): 12.07, 9.31, 1.68						
Atom	Wyckoff Site	x/a	y/b	z/c	Occ.	U_{iso} / Å^2
Ag1	1a	0	0	0	1.00	0.0750
Ag2	2d	0.3333	0.6667	-0.3309(2)	0.940(1)	0.0119(4)
Ag3	2d	0.3333	0.6667	0.1608(1)	0.060(1)	0.0147(3)
Bi1	1b	0	0	0.5	1.00	0.0011(1)
Bi2	2d	0.3333	0.6667	0.1608(1)	0.940(1)	0.0147(3)
Bi3	2d	0.3333	0.6667	-0.3309(2)	0.060(1)	0.0119(4)
Se1	2d	0	0	0.2506(2)	1.00	0.0426(4)
Se2	2d	0.3333	0.6667	-0.0757(2)	1.00	0.0426(4)
Se3	2d	0.3333	0.6667	0.4130(3)	1.00	0.0426(4)

Table S2. Crystallographic data (atomic coordinates, occupancy, and U_{iso}) of $Ag_{0.99}BiSe_2$, obtained from Rietveld refinements of X-ray synchrotron diffraction.

$Ag_{0.99}BiSe_2$ structure from X-ray powder diffraction (space group $P\bar{3}m1$) *a* = 4.1907(1) Å; *c* = 19.6625(3) Å; 15.8 % $R\bar{3}m$; 1.7 % Bi_2Se_3 Fit residuals (R_{wp}, R_{exp}, χ^2): 13.14, 9.99, 1.73						
Atom	Wyckoff Site	x/*a*	y/*b*	z/*c*	Occ.	U_{iso} / Å^2
Ag1	1*a*	0	0	0	1.00	0.0750
Ag2	2*d*	0.3333	0.6667	-0.3312(2)	0.980(1)	0.0109(5)
Ag3	2*d*	0.3333	0.6667	0.1612(1)	0.020(1)	0.0107(5)
Bi1	1*b*	0	0	0.5	1.00	0.0037(5)
Bi2	2*d*	0.3333	0.6667	0.1612(1)	0.980(1)	0.0107(5)
Bi3	2*d*	0.3333	0.6667	-0.3312(2)	0.020(1)	0.0109(5)
Se1	2*d*	0	0	0.2519(2)	1.00	0.0428(5)
Se2	2*d*	0.3333	0.6667	-0.0761(3)	1.00	0.0428(5)
Se3	2*d*	0.3333	0.6667	0.4148(3)	1.00	0.0428(5)

Table S3. Crystallographic data (atomic coordinates, occupancy, and U_{iso}) of $Ag_{0.98}BiSe_2$, obtained from Rietveld refinements of X-ray synchrotron diffraction.

$Ag_{0.98}BiSe_2$ structure from X-ray powder diffraction (space group $P\bar{3}m1$) a = 4.1962(1) Å; c = 19.6462(3) Å; 14.9 % $R\bar{3}m$ Fit residuals (R_{wp}, R_{exp}, χ^2): 14.27, 9.17, 2.42						
Atom	Wyckoff Site	x/a	y/b	z/c	Occ.	U_{iso} / Å^2
Ag1	1a	0	0	0	1.00	0.0750
Ag2	2d	0.3333	0.6667	-0.3304(2)	0.987(1)	0.0066(4)
Ag3	2d	0.3333	0.6667	0.1609(1)	0.013(1)	0.0070(2)
Bi1	1b	0	0	0.5	1.00	0.0035(4)
Bi2	2d	0.3333	0.6667	0.1609(1)	0.987(1)	0.0070(2)
Bi3	2d	0.3333	0.6667	-0.3304(2)	0.013(1)	0.0066(4)
Se1	2d	0	0	0.2526(2)	1.00	0.0448(4)
Se2	2d	0.3333	0.6667	-0.0754(2)	1.00	0.0448(4)
Se3	2d	0.3333	0.6667	0.4154(3)	1.00	0.0448(4)

Table S4. Crystallographic data (atomic coordinates, occupancy, and U_{iso}) of $Ag_{0.95}BiSe_2$, obtained from Rietveld refinements of X-ray synchrotron diffraction.

$Ag_{0.95}BiSe_2$ structure from X-ray powder diffraction (space group $P\bar{3}m1$) *a* = 4.19002(5) Å; *c* = 19.6563(2) Å; 11.0 % $R\bar{3}m$ Fit residuals (R_{wp}, R_{exp}, χ^2): 12.40, 9.35, 1.76						
Atom	Wyckoff Site	x/*a*	y/*b*	z/*c*	Occ.	U_{iso} / Å^2
Ag1	1*a*	0	0	0	1.00	0.0750
Ag2	2*d*	0.3333	0.6667	-0.3312(2)	1.00	0.0095(4)
Bi1	1*b*	0	0	0.5	1.00	0.0012(3)
Bi2	2*d*	0.3333	0.6667	0.1611(1)	1.00	0.0222(5)
Se1	2*d*	0	0	0.2513(2)	1.00	0.0554(4)
Se2	2*d*	0.3333	0.6667	-0.0752(3)	1.00	0.0554(4)
Se3	2*d*	0.3333	0.6667	0.4129(3)	1.00	0.0554(4)

Table S5. Crystallographic data (atomic coordinates, occupancy, and U_{iso}) of $Ag_{0.93}BiSe_2$, obtained from Rietveld refinements of X-ray synchrotron diffraction.

$Ag_{0.93}BiSe_2$ structure from X-ray powder diffraction (space group $P\bar{3}m1$) a = 4.1951(1) Å; c = 19.6570(2) Å; 16.1 % $R\bar{3}m$; 1.4 % Bi_4Se_3 Fit residuals (R_{wp}, R_{exp}, χ^2): 11.18, 8.89, 1.58						
Atom	Wyckoff Site	x/a	y/b	z/c	Occ.	U_{iso} / Å^2
Ag1	1a	0	0	0	1.00	0.0750
Ag2	2d	0.3333	0.6667	-0.3309(2)	1.00	0.0078(6)
Bi1	1b	0	0	0.5	1.00	0.0011(4)
Bi2	2d	0.3333	0.6667	0.1609(1)	1.00	0.0189(6)
Se1	2d	0	0	0.2507(2)	1.00	0.0478(5)
Se2	2d	0.3333	0.6667	-0.0766(3)	1.00	0.0478(5)
Se3	2d	0.3333	0.6667	0.4135(3)	1.00	0.0478(5)