Supplementary information

The development of approach to the precision determination of the thermal strain tensor elements for single crystals on the example of *t*-$Ag_{0.8}Li_{0.2}InSe_2$

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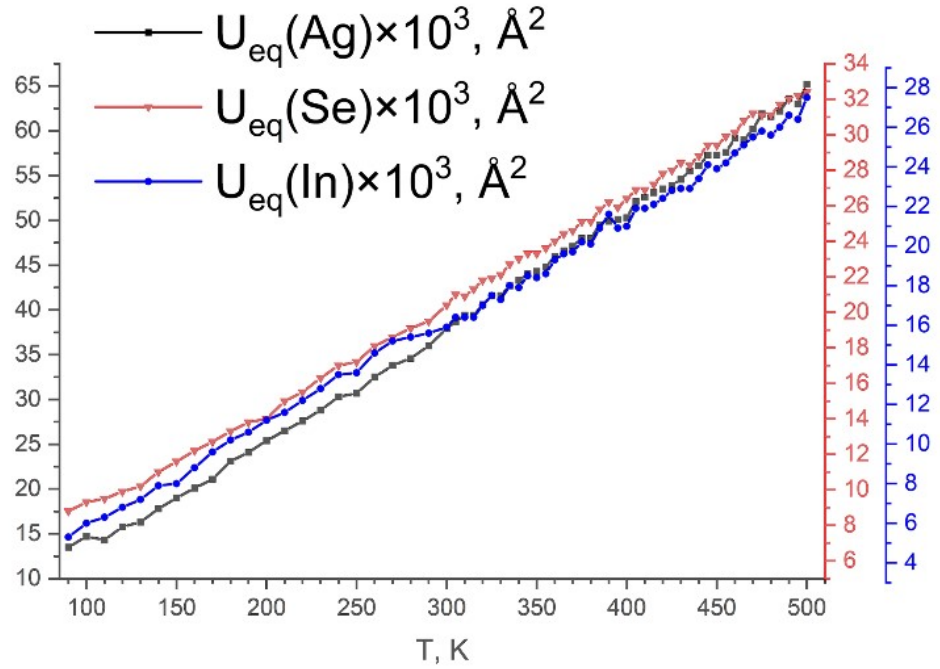
Table S1 *t*-$Ag_{0.8}Li_{0.2}InSe_2$ sample **1** crystallographic parameters and the results of structure refinement

Crystal data		
Chemical formula	$Ag_{0.795}InLi_{0.205}Se_2$	$Ag_{0.796}InLi_{0.204}Se_2$
M_r	359.92	359.92
Crystal system, space group	Tetragonal, *I*-42*d*	Tetragonal, *I*-42*d*
Temperature (K)	150	300
a, *c* (Å)	6.0640 (3), 11.6831 (7)	6.07290 (14), 11.6732 (4)
V (Å^3)	429.61 (5)	430.51 (2)
Z	4	4
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	25.73	25.68
Crystal size (mm)	0.12 × 0.12 × 0.06	
Data collection		
Diffractometer	Bruker D8 VENTURE	Bruker D8 VENTURE
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1144 before and 0.0368 after correction. The Ratio of minimum to maximum transmission is 0.6163. The λ/2 correction factor is Not present.	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0891 before and 0.0425 after correction. The Ratio of minimum to maximum transmission is 0.6306. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.460, 0.747	0.471, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1250, 413, 337	1890, 517, 411
R_{int}	0.019	0.023
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.768	0.834
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.019, 0.045, 1.08	0.020, 0.054, 1.10
No. of reflections	413	517
No. of parameters	12	12
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.72, −0.89	0.71, −0.59
Absolute structure	Flack x determined using 132 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 164 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.03 (2)	0.002 (19)

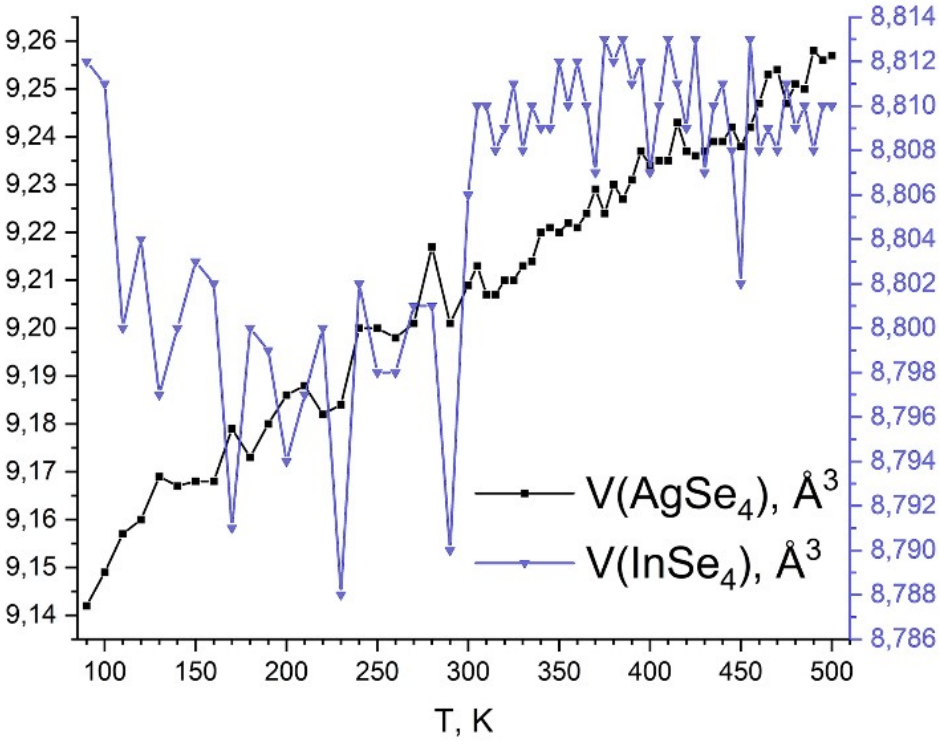
Table S2 *t*-$Ag_{0.8}Li_{0.2}InSe_2$ sample **2** and **3** crystallographic parameters and the results of structure refinement

Crystal data		
Sample number	Sample **2**	Sample **3**
Chemical formula	$Ag_{0.793}InLi_{0.207}Se_2$	$Ag_{0.790}InLi_{0.210}Se_2$
M_r	359.67	359.41
Crystal system, space group	Tetragonal, *I*-42*d*	Tetragonal, *I*-42*d*
Temperature (K)	150	300
a, *c* (Å)	6.0658 (3), 11.6925 (7)	6.07490 (14), 11.6869 (5)
V (Å^3)	430.21 (5)	431.30 (3)
Z	4	4
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	25.68	25.61
Crystal size (mm)	0.15 × 0.15 × 0.06	0.25× 0.25 × 0.2
Data collection		
Diffractometer	Bruker D8 VENTURE	Bruker D8 VENTURE
Absorption correction	Multi-scan SADABS2016/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0817 before and 0.0338 after correction. The Ratio of minimum to maximum transmission is 0.5634. The λ/2 correction factor is Not present.	Numerical *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1553 before and 0.0704 after correction. The Ratio of minimum to maximum transmission is 0.1109. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.421, 0.747	0.017, 0.149
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	987, 410, 338	3452, 520, 395
R_{int}	0.013	0.052
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.771	0.833
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.016, 0.047, 1.14	0.040, 0.120, 1.05
No. of reflections	410	520
No. of parameters	12	12
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.75, −0.46	1.01, −1.42
Absolute structure	Flack x determined using 132 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Classical Flack method preferred over Parsons because s.u. lower.
Absolute structure parameter	0.00 (2)	−0.07 (6)

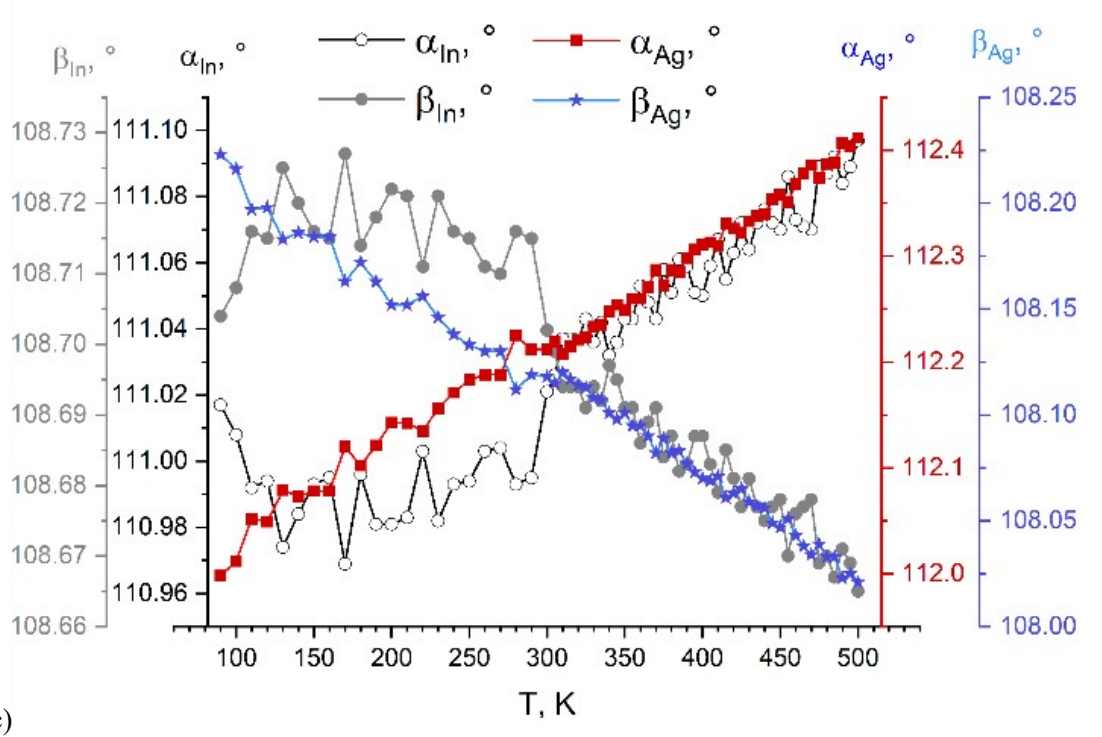
Fig. S1 *t*-$Ag_{0.8}Li_{0.2}InSe_2$ crystal structure parameters changes in the 90-500 K range according to the SC-XRD data: the equivalent parameter of the atomic displacement for the main atoms (a); the volumes of the coordination tetrahedra $AgSe_4$ and $InSe_4$ (b); the angles in the structure according to Fig. 7 (c, d).



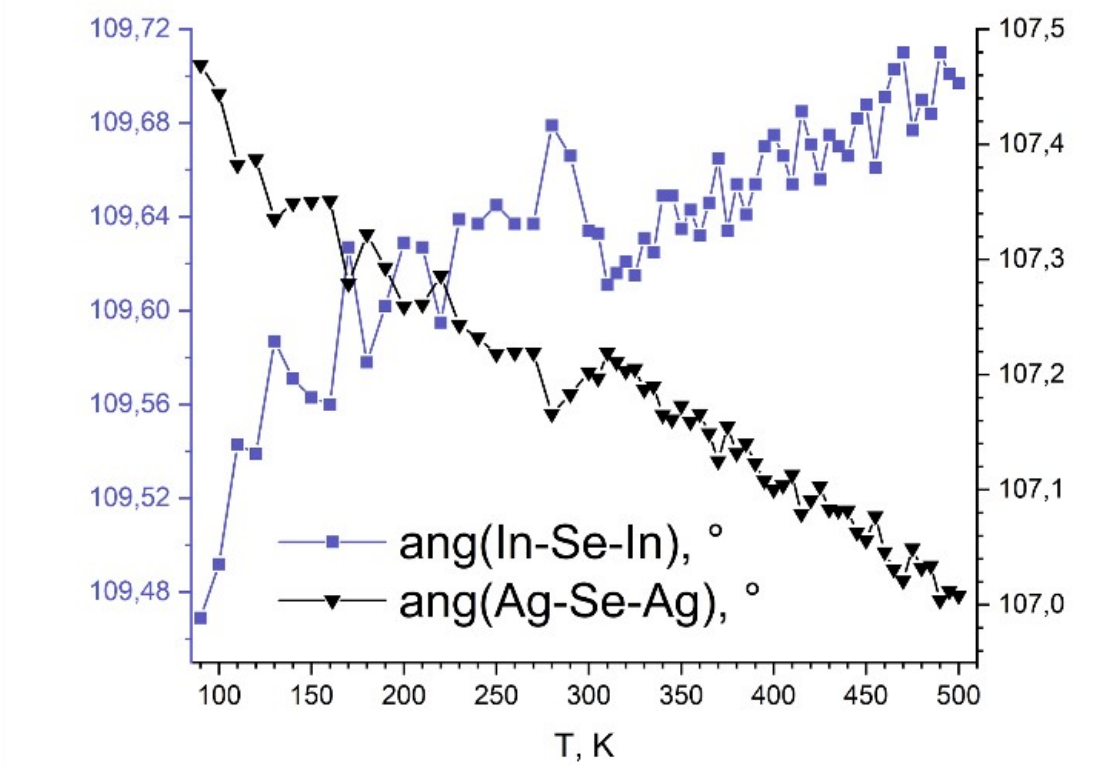
a)



b)


βIn, °
αIn, °
αIn, °
αAg, °
βIn, °
βAg, °
αAg, °
βAg, °
108.73
108.72
108.71
108.70
108.69
108.68
108.67
108.66
111.10
111.08
111.06
111.04
111.02
111.00
110.98
110.96
112.4
112.3
112.2
112.1
112.0
108.25
108.20
108.15
108.10
108.05
108.00
100
150
200
250
300
350
400
450
500
T, K

c)


109,72
109,68
109,64
109,60
109,56
109,52
109,48
107,5
107,4
107,3
107,2
107,1
107,0
ang(In-Se-In), °
ang(Ag-Se-Ag), °
100
150
200
250
300
350
400
450
500
T, K

d)

Table S3 The results of reflexes processing when refining the UCP by doublet reflexes of the external Si standard (T = 300 K)

h k l	2θcalc, °	X, pix.	Y, pix.	2θexp, °	*a*, *c*, Å
Crystal **1**. *D*=109.07, $2\theta_D$ = -85°					
$K\alpha_1(1\ -5\ 9)_{Si}$	84.987	387.66	505.29		
$K\alpha_1(10\ 6\ 0)_{\mathbf{1}}$	86.009[A]	397.87	505.33	85.705	6.0813(6)[B]
$K\alpha_2(1\ -5\ 9)_{Si}$	85.623	396.70	504.88		
Crystal **1**. *D*=109.07, $2\theta_D$ = -85°					
$K\alpha_1(11\ 1\ 1)_{Si}$	92.813	382.52	502.86		
$K\alpha_1(0\ 0\ 24)_{\mathbf{1}}$	93.531[A]	392.53	506.56	93.523	11.684(1)
$K\alpha_1(11\ 1\ 1)_{Si}$	93.543	392.81	503.12		
Crystal **2**. *D*=109.07, $2\theta_D$ = -85°					
$K\alpha_1(1\ -5\ 9)_{Si}$	84.987	385.04	505.55		
$K\alpha_1(10\ 6\ 0)_{\mathbf{2}}$	85.977[A]	395.27	504.87	85.714	6.0808(6)
$K\alpha_2(1\ -5\ 9)_{Si}$	85.623	393.99	505.75		
Crystal **2**. *D*=109.07, $2\theta_D$ = -85°					
$K\alpha_1(11\ 1\ 1)_{Si}$	92.813	382.52	502.86		
$K\alpha_1(0\ 0\ 24)_{\mathbf{2}}$	93.433[A]	392.54	506.78	93.524	11.684(1)
$K\alpha_1(11\ 1\ 1)_{Si}$	93.543	392.81	503.12		
Crystal $Ag_{0.63}Li_{0.37}InSe_2$. *D*=109.07, $2\theta_D$ = -85°					
$K\alpha_1(1\ -5\ 9)_{Si}$	84.987	387.28	505.94		
$K\alpha_1(6\ -10\ 0)$	86.157[A]	403.67	506.89	86.132	6.0570(6)
$K\alpha_1(0\ 8\ -16)$	85.002[A]	388.03	507.90	85.039	11.648(1)
$K\alpha_2(1\ -5\ 9)_{Si}$	85.623	396.38	506.08		

A – calculated by the results of single crystal XRD
B – absolute errors were calculated for Δθ=0.005°

Fig. S2 The dependence of the relative error in determining UCP by the "Doublet" method on the vertically displacement of studied diffraction peak, based on the experiment with Si .The level of relative error in UCP determination calculated from the goniometer positioning error is shown by a red dotted line.