



Substitution of indium for chromium in $\text{TlIn}_{5-x}\text{Cr}_x\text{Se}_8$: crystal structure of $\text{TlIn}_{4.811(5)}\text{Cr}_{0.189(5)}\text{Se}_8$

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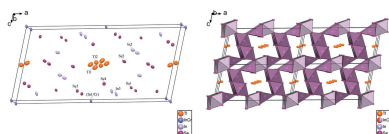
The new thallium penta(indium/chromium) octaselenide, $\text{TlIn}_{4.811(5)}\text{Cr}_{0.189(5)}\text{Se}_8$, has been synthesized by solid-state reaction. It crystallizes isotypically with TlIn_5Se_8 in the space group $C2/m$. Although the two Tl positions are disordered and only partially occupied, no Tl deficiency was observed. The insertion of chromium in the structure has been confirmed by EDS analysis. Chromium substitutes indium exclusively at one of three In sites, *viz.* at one of the positions with site symmetry $2/m$ (Wyckoff position $2a$). In the crystal structure, edge-sharing InSe_6 octahedra, and $(\text{In,Cr})\text{Se}_6$ octahedra and InSe_4 tetrahedra make up two types of columns that are linked into a framework in which two different types of channels parallel to $[010]$ are present. The Tl atoms are located in the larger of the channels, whereas the other, smaller channel remains unoccupied.

1. Chemical context

This study is part of an on-going project focused on low-dimensional chalcogenides with low thermal conductivity. Quasi one-dimensional networks are of great interest for thermoelectric applications. Such structures can combine structural disorder, responsible for scattering of phonons, to an electronically conductive network.

Recently, low thermal conductive compounds belonging to the family of pseudo-hollandites were studied. A thermoelectric figure of merit up to $ZT = 0.5$ at 800 K was found for TlCr_5Se_8 (Takahashi *et al.*, 2013). This discovery inspired further studies on this class of materials. Pseudo-hollandites are compounds with general formula AM_5X_8 , (A = alkali metal, alkaline earth metal, Tl; M = V, Ti, Cr; X = S, Se, Te), the structures of which are made up from CdI_2 -type layers and double chains of MX_6 octahedra sharing edges and faces in such a way that channels are created along one axis in which the A cations are located. Monoclinic TlCr_5Se_8 and the related triclinic compound $\text{Ba}_{0.5}\text{Cr}_5\text{Se}_8$ have thermal conductivities well below $1 \text{ W m}^{-1} \text{ K}^{-1}$ from room temperature to 873 K (Lefèvre *et al.*, 2015, 2016). As part of our project, we successfully synthesized a solid solution of $\text{TlV}_{5-x}\text{Cr}_x\text{Se}_8$ ($x = 0, 1, 2, 3, 4, 5$) and studied the magnetism and thermoelectric properties of TlV_5Se_8 (Maier *et al.*, 2015).

Working on a similar compound, monoclinic TlIn_5Se_8 , we attempted to synthesize a solid solution $\text{TlIn}_{5-x}\text{Cr}_x\text{Se}_8$. Initially, the nominal composition $\text{TlIn}_4\text{CrSe}_8$ was chosen so that chromium fully substitutes indium at the octahedral site (Wyckoff position $2a$) of TlIn_5Se_8 . Here we present the structure of one compound of the solid solution series



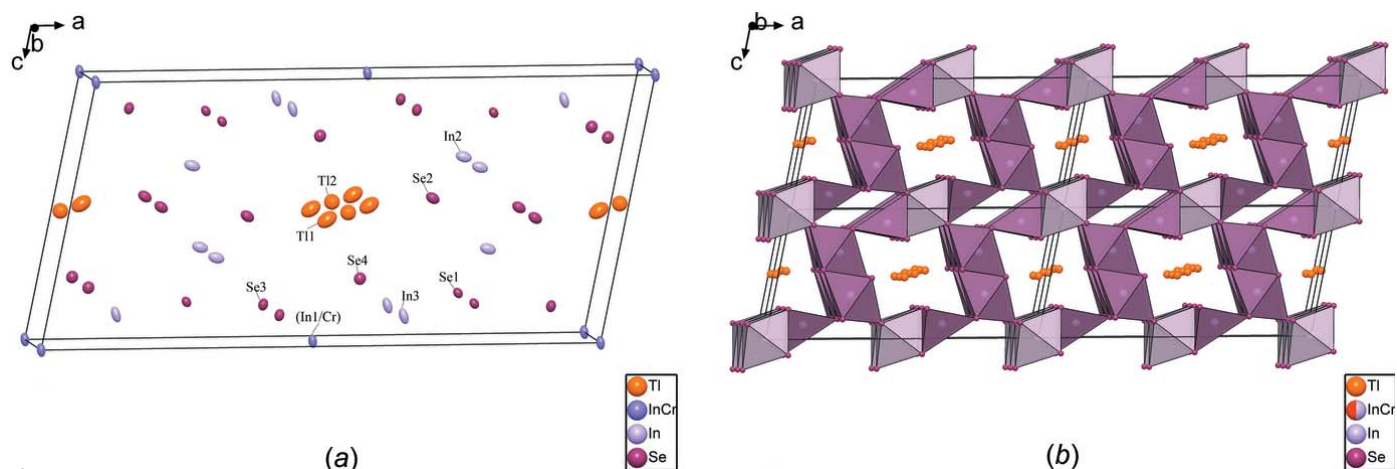


Figure 1 The crystal structure of $\text{TIIn}_{4.811(5)}\text{Cr}_{0.189(5)}\text{Se}_8$. (a) Representation by atoms displayed with displacement ellipsoids at the 50% probability level; (b) polyhedral representation.

$\text{TIIn}_{5-x}\text{Cr}_x\text{Se}_8$ ($x = 0.189$) with only a partial substitution of indium for chromium at this site.

2. Structural commentary

The composition of the crystals as determined from the refinement is in good agreement with the EDS analysis. The refined structure is represented in Fig. 1, both as individual atoms and in a polyhedral representation. All atoms in the asymmetric unit (two TI, one mixed-occupied In/Cr, two In and four Se sites) are located on special positions. Except TI2 and mixed-occupied (In1/Cr) on positions with site symmetry $2/m$ (Wyckoff positions $2d$ and $2a$, respectively), all other atoms are located on a mirror plane ($4i$).

Indium atoms are found in octahedral (In1, In2) and tetrahedral (In3) environments by selenium atoms. Only one of the indium atoms, In1, shares its position with chromium in an octahedral environment. The $(\text{In1,Cr})\text{Se}_6$ and In2Se_6 octahedra form two types of columns. One column is made up only of edge-sharing In2Se_6 octahedra in a zigzag shape. The second column is made up of alternating $(\text{In1/Cr})\text{Se}_6$ octahedra and In3Se_4 tetrahedra connected by edge-sharing, likewise in a zigzag shape. These two building units are linked together to form a framework in which two types of channels

propagating parallel to $[010]$ are present. One of the channels hosts the two partly occupied TI atoms, while the other is smaller and thus empty. Compared to the pseudo-hollandite network, the infinite planes are broken into columns in the title structure, leaving a supplementary channel at the junction of the columns and the double chains.

The existence of the title solid solution is in agreement with the decrease or increase of unit-cell parameters of $\text{TIIn}_{5-x}\text{Cr}_x\text{Se}_8$ from $x = 0$ (Walther & Deiseroth, 1998) to $x = 5$ (Klepp & Boller, 1983), as explicated in Fig. 2*a*. Further, the decrease in the determined metal-to-metal and metal-to-selenium distances shows a clear trend in agreement with the increase of the chromium content (Fig. 2*b,c*).

3. Synthesis and crystallization

To prevent oxidation of reactants and products, all manipulations were performed under inert gas or vacuum (glove box or sealed containers). The elements, Cr (powder, 325 mesh, 99%), In (teardrops, 4 mm, 99.9%) and Se (shots, 99.999%), all from Alfa Aesar, were used as received; TI (granules, 99.99%), as well from Alfa Aesar, received in water, was first rinsed and dried before being stored in a glovebox. The elements TI, In, Cr and Se in the molar ratio 1:4:1:8 were

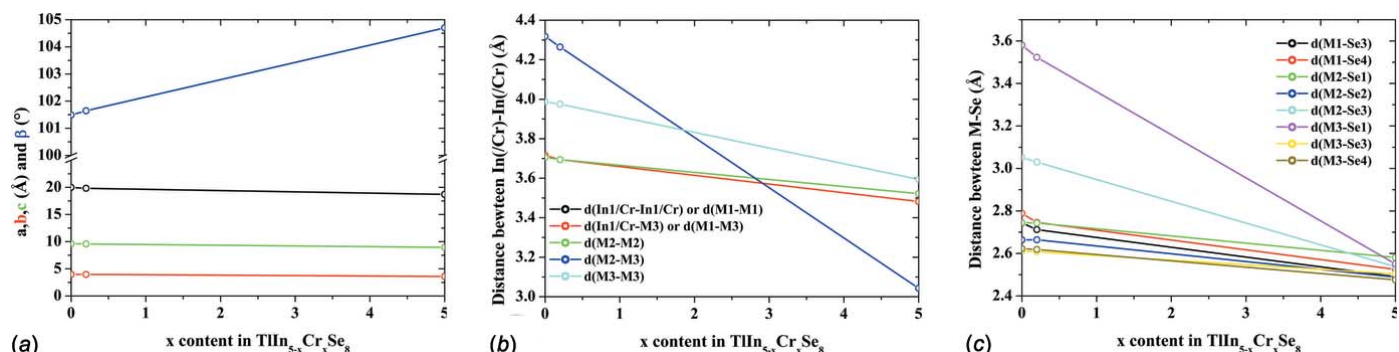


Figure 2 Evolution of (a) the unit-cell parameters, (b) $M-M$ distances and (c) $M-Se$ distances depending on x in the $\text{TIIn}_{5-x}\text{Cr}_x\text{Se}_8$ solid solution series.

Table 1
Experimental details.

Crystal data	
Chemical formula	TlIn _{4.811} Cr _{0.189} Se ₈
M_r	1398.3
Crystal system, space group	Monoclinic, $C2/m$
Temperature (K)	293
a, b, c (Å)	19.8257 (18), 3.9754 (4), 9.5881 (9)
β (°)	101.645 (5)
V (Å ³)	740.13 (12)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	37.98
Crystal size (mm)	0.13 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Numerical (SADABS; Bruker, 2004)
T_{\min}, T_{\max}	0.405, 0.747
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	5647, 1537, 1181
R_{int}	0.028
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.770
Refinement	
$R[F > 3\sigma(F)], wR(F), S$	0.030, 0.031, 1.34
No. of reflections	1537
No. of parameters	50
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.41, -1.69

Computer programs: APEX2 and SAINT (Bruker, 2004), SUPERFLIP (Palatinus & Chapuis, 2007), DIAMOND (Brandenburg & Putz, 2014), JANA2006 (Petříček *et al.*, 2014) and publCIF (Westrip, 2010).

loaded directly in a fused silica tube that was subsequently evacuated and flame sealed. The mixture was first heated up to 723 K within 7 h for half a day, and then to 1073 K in 7 h for half a day. The mixture was then cooled down to room temperature in 48 h. An intermediate annealing process at 873 K for 15 h was performed. Single crystals were extracted from the bulk.

The bulk sample quality was checked by means of X-ray powder diffraction using a X-Pert Pro Panalytical diffractometer (Cu $K\alpha_{1,2}$ radiations) equipped with a PIXCEL detector. Phase identification was performed with *X'Pert HighScore plus* (Panalytical, 2009). Phase analysis using X-ray powder diffraction revealed at first sight TlCr₅Se₈ (Klepp & Boller, 1983) and TlIn₅Se₈ (Walther & Deiseroth, 1998). However, the Bragg positions of these reflections were clearly shifted, pointing to the presence of a TlIn_{5-x}Cr_xSe₈ solid solution.

Energy Dispersive X-Ray Spectroscopy (EDS) analyses were also performed to check the composition using a scanning electron microscope (SEM; ZEISS Supra 55, 15 kV). Analysis on basis of nine measured crystallites confirmed the presence of four elements, with a determined average molar composition of Tl 1.05; In 4.54; Cr 0.46; Se 9.1.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Structure solution using *SUPERFLIP* (Palatinus & Chapuis, 2007) led to one thallium site, three indium sites and four selenium sites. Refinement of Tl1 in position (0.5,0,0.5) resulted in large anisotropic displacement parameters. As previously reported, Tl1 usually is located at a partly occupied position around the center position with approximate coordinates of (0.46, 0, 0.52) (Walther & Deiseroth, 1998). Consideration of the split model (in addition, the In1 site occupancy refined to 0.81 while other indium sites were modelled as fully occupied) led to much more reasonable displacement parameters and improved reliability factors. At that step, the reliability factors were: GOF(all reflections) = 2.42 and wR (all reflections) = 0.056, while the maximum and minimum electron densities were +10.28 and -6.03 e⁻ Å⁻³.

The insertion of chromium in the structure has been confirmed by EDS analysis. Consideration of a mixed-occupied In/Cr site for the original In1 position (same coordinates and anisotropic displacement parameters for the two atoms and full occupation for this site) led to a further improvement of reliability factors [GOF (all) = 2.06 and wR (all) = 0.0476] and a decrease of the residual electron densities to +9.71 and -5.83 e⁻ Å⁻³. The maximum electron density was found on position (0, 0.5, 0.5). This position is between the partially occupied Tl1 atoms. Thus, a second partially occupied thallium atom, Tl2, was introduced. The two thallium sites are non-simultaneously occupied. The displacement parameter of Tl2 was modelled as isotropic due to its low occupancy compared to Tl1. Adding this second Tl site significantly reduced the residual electron density to final values of +1.41 and -1.69 e⁻ Å⁻³. These density peaks are found at 0.82 and 0.73 Å, respectively, from atoms Se2 and In3.

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE* (Bruker, 2004); program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2014); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2014); software used to prepare material for publication: *JANA2006* (Petříček *et al.*, 2014) and *publCIF* (Westrip, 2010).

Thallium penta(indium/chromium) octaselenide

Crystal data

$\text{TlIn}_{4.811}\text{Cr}_{0.189}\text{Se}_8$
 $M_r = 1398.3$
 Monoclinic, $C2/m$
 Hall symbol: $-C\ 2y$
 $a = 19.8257\ (18)\ \text{Å}$
 $b = 3.9754\ (4)\ \text{Å}$
 $c = 9.5881\ (9)\ \text{Å}$
 $\beta = 101.645\ (5)^\circ$
 $V = 740.13\ (12)\ \text{Å}^3$
 $Z = 2$

$F(000) = 1187$
 $D_x = 6.274\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{Å}$
 Cell parameters from 2692 reflections
 $\theta = 2.7\text{--}32.8^\circ$
 $\mu = 37.98\ \text{mm}^{-1}$
 $T = 293\ \text{K}$
 Irregular, black
 $0.13 \times 0.11 \times 0.10\ \text{mm}$

Data collection

Bruker APEXII CCD area detector
 diffractometer
 Radiation source: X-ray tube
 Graphite monochromator
 Detector resolution: $8.3333\ \text{pixels mm}^{-1}$
 ω and φ scans
 Absorption correction: numerical
 (*SADABS*; Bruker, 2004)
 $T_{\min} = 0.405$, $T_{\max} = 0.747$

5647 measured reflections
 1537 independent reflections
 1181 reflections with $I > 3\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 33.2^\circ$, $\theta_{\min} = 2.1^\circ$
 $h = -30 \rightarrow 26$
 $k = -5 \rightarrow 6$
 $l = -12 \rightarrow 14$

Refinement

Refinement on F
 $R[F > 3\sigma(F)] = 0.030$
 $wR(F) = 0.031$
 $S = 1.34$
 1537 reflections
 50 parameters
 0 restraints

4 constraints
 Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(F) + 0.0001F^2)$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 1.41\ \text{e Å}^{-3}$
 $\Delta\rho_{\min} = -1.69\ \text{e Å}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Tl1	0.46491 (5)	0	0.52551 (8)	0.0407 (3)	0.4631 (16)
Tl2	0	0.5	0.5	0.032 (2)*	0.074 (3)
In1	0	0	0	0.0155 (2)	0.811 (5)
Cr	0	0	0	0.0155 (2)	0.189 (5)
In2	0.28034 (3)	0	0.66298 (5)	0.02131 (15)	
In3	0.36250 (2)	0	0.10972 (5)	0.02052 (15)	
Se1	0.24067 (3)	0	0.15323 (6)	0.01295 (17)	
Se2	0.16279 (4)	0	0.47058 (7)	0.0197 (2)	
Se3	0.58556 (3)	0	0.11945 (6)	0.01640 (19)	
Se4	0.06189 (3)	0	0.76833 (7)	0.01829 (19)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tl1	0.0434 (6)	0.0352 (4)	0.0376 (4)	0	−0.0058 (3)	0
In1	0.0110 (4)	0.0129 (4)	0.0240 (4)	0	0.0069 (3)	0
Cr	0.0110 (4)	0.0129 (4)	0.0240 (4)	0	0.0069 (3)	0
In2	0.0346 (3)	0.0138 (2)	0.01692 (19)	0	0.00868 (19)	0
In3	0.0158 (2)	0.0166 (2)	0.0327 (3)	0	0.01323 (19)	0
Se1	0.0129 (3)	0.0129 (3)	0.0142 (3)	0	0.0053 (2)	0
Se2	0.0256 (4)	0.0174 (3)	0.0183 (3)	0	0.0094 (2)	0
Se3	0.0121 (3)	0.0179 (3)	0.0187 (3)	0	0.0019 (2)	0
Se4	0.0189 (3)	0.0153 (3)	0.0204 (3)	0	0.0035 (2)	0

Geometric parameters (\AA , $^\circ$)

Tl1—Tl1 ⁱ	3.9754 (8)	Cr—Se3 ^{xiii}	2.7122 (5)
Tl1—Tl1 ⁱⁱ	3.9754 (8)	Cr—Se4 ^{xiv}	2.7460 (8)
Tl1—Tl1 ⁱⁱⁱ	1.5654 (15)	Cr—Se4 ^{viii}	2.7460 (8)
Tl1—Tl2 ^{iv}	0.7827 (11)	In2—In2 ⁱ	3.9754 (8)
Tl1—Se2 ^v	3.2249 (11)	In2—In2 ⁱⁱ	3.9754 (8)
Tl1—Se2 ^{vi}	3.2249 (11)	In2—In2 ^v	3.6944 (8)
Tl1—Se3 ⁱⁱⁱ	3.7369 (13)	In2—In2 ^{vi}	3.6944 (8)
Tl1—Se4 ^{iv}	3.3558 (9)	In2—Se1 ^v	2.7433 (6)
Tl1—Se4 ^{vii}	3.3558 (9)	In2—Se1 ^{vi}	2.7433 (6)
Tl1—Se4 ^v	3.4010 (9)	In2—Se2	2.6644 (9)
Tl1—Se4 ^{vi}	3.4010 (9)	In2—Se2 ^v	2.7286 (7)
Tl2—Tl2 ⁱ	3.9754 (8)	In2—Se2 ^{vi}	2.7286 (7)
Tl2—Tl2 ⁱⁱ	3.9754 (8)	In2—Se3 ⁱⁱⁱ	3.0300 (9)
Tl2—Se2	3.8489 (8)	In3—In3 ⁱ	3.9754 (8)
Tl2—Se2 ⁱⁱ	3.8489 (8)	In3—In3 ⁱⁱ	3.9754 (8)
Tl2—Se2 ^{viii}	3.8489 (8)	In3—Se1	2.5328 (9)
Tl2—Se2 ^{ix}	3.8489 (8)	In3—Se1 ^{xii}	3.5227 (7)
Tl2—Se4	3.2865 (7)	In3—Se1 ^{xiii}	3.5227 (7)
Tl2—Se4 ⁱⁱ	3.2865 (7)	In3—Se3 ^{xv}	2.6080 (9)

Tl2—Se4 ^{viii}	3.2865 (7)	In3—Se4 ^v	2.6186 (6)
Tl2—Se4 ^{ix}	3.2865 (7)	In3—Se4 ^{vi}	2.6186 (6)
In1—In1 ⁱ	3.9754 (8)	Se1—Se1 ⁱ	3.9754 (8)
In1—In1 ⁱⁱ	3.9754 (8)	Se1—Se1 ⁱⁱ	3.9754 (8)
In1—Cr ⁱ	3.9754 (8)	Se1—Se1 ^{xii}	3.6278 (9)
In1—Cr	0	Se1—Se1 ^{xiii}	3.6278 (9)
In1—Cr ⁱⁱ	3.9754 (8)	Se1—Se2	3.6795 (11)
In1—In3 ^x	3.6941 (6)	Se1—Se3 ^x	3.6207 (9)
In1—In3 ^{xi}	3.6941 (6)	Se1—Se3 ^{xi}	3.6207 (9)
In1—In3 ^{xii}	3.6941 (6)	Se2—Se2 ⁱ	3.9754 (8)
In1—In3 ^{xiii}	3.6941 (6)	Se2—Se2 ⁱⁱ	3.9754 (8)
In1—Se3 ^x	2.7122 (5)	Se2—Se2 ^v	3.9294 (10)
In1—Se3 ^{xi}	2.7122 (5)	Se2—Se2 ^{vi}	3.9294 (10)
In1—Se3 ^{xii}	2.7122 (5)	Se2—Se3 ^x	3.9432 (9)
In1—Se3 ^{xiii}	2.7122 (5)	Se2—Se3 ^{xi}	3.9432 (9)
In1—Se4 ^{xiv}	2.7460 (8)	Se2—Se4	3.8022 (11)
In1—Se4 ^{viii}	2.7460 (8)	Se3—Se3 ⁱ	3.9754 (8)
Cr—Cr ⁱ	3.9754 (8)	Se3—Se3 ⁱⁱ	3.9754 (8)
Cr—Cr ⁱⁱ	3.9754 (8)	Se3—Se3 ^{xv}	3.6905 (11)
Cr—In3 ^x	3.6941 (6)	Se3—Se4 ^{xvi}	3.8558 (10)
Cr—In3 ^{xi}	3.6941 (6)	Se3—Se4 ^{xvii}	3.8558 (10)
Cr—In3 ^{xii}	3.6941 (6)	Se3—Se4 ^v	3.8633 (10)
Cr—In3 ^{xiii}	3.6941 (6)	Se3—Se4 ^{vi}	3.8633 (10)
Cr—Se3 ^x	2.7122 (5)	Se4—Se4 ⁱ	3.9754 (8)
Cr—Se3 ^{xi}	2.7122 (5)	Se4—Se4 ⁱⁱ	3.9754 (8)
Cr—Se3 ^{xii}	2.7122 (5)		
Tl1 ⁱ —Tl1—Tl1 ⁱⁱ	180.0 (5)	In3 ^{xii} —Se1—Se1 ^{xiii}	82.466 (16)
Tl1 ⁱ —Tl1—Tl1 ⁱⁱⁱ	90.00 (2)	In3 ^{xii} —Se1—Se2	108.174 (19)
Tl1 ⁱ —Tl1—Tl2 ^{iv}	90.00 (2)	In3 ^{xii} —Se1—Se3 ^x	42.799 (14)
Tl1 ⁱ —Tl1—Se2 ^v	51.949 (18)	In3 ^{xii} —Se1—Se3 ^{xi}	83.442 (16)
Tl1 ⁱ —Tl1—Se2 ^{vi}	128.05 (3)	In3 ^{xiii} —Se1—Se1 ⁱ	124.351 (15)
Tl1 ⁱ —Tl1—Se3 ⁱⁱⁱ	90.000 (18)	In3 ^{xiii} —Se1—Se1 ⁱⁱ	55.649 (10)
Tl1 ⁱ —Tl1—Se4 ^{iv}	53.678 (14)	In3 ^{xiii} —Se1—Se1 ^{xii}	82.466 (16)
Tl1 ⁱ —Tl1—Se4 ^{vii}	126.32 (2)	In3 ^{xiii} —Se1—Se1 ^{xiii}	41.459 (14)
Tl1 ⁱ —Tl1—Se4 ^v	54.236 (14)	In3 ^{xiii} —Se1—Se2	108.174 (19)
Tl1 ⁱ —Tl1—Se4 ^{vi}	125.76 (2)	In3 ^{xiii} —Se1—Se3 ^x	83.442 (16)
Tl1 ⁱⁱ —Tl1—Tl1 ⁱⁱⁱ	90.00 (2)	In3 ^{xiii} —Se1—Se3 ^{xi}	42.799 (14)
Tl1 ⁱⁱ —Tl1—Tl2 ^{iv}	90.00 (2)	Se1 ⁱ —Se1—Se1 ^{xii}	56.776 (11)
Tl1 ⁱⁱ —Tl1—Se2 ^v	128.05 (3)	Se1 ⁱ —Se1—Se1 ^{xiii}	123.224 (17)
Tl1 ⁱⁱ —Tl1—Se2 ^{vi}	51.949 (18)	Se1 ⁱ —Se1—Se3 ^x	56.703 (11)
Tl1 ⁱⁱ —Tl1—Se3 ⁱⁱⁱ	90.000 (18)	Se1 ⁱ —Se1—Se3 ^{xi}	123.297 (17)
Tl1 ⁱⁱ —Tl1—Se4 ^{iv}	126.32 (2)	Se1 ⁱⁱ —Se1—Se1 ^{xii}	123.224 (17)
Tl1 ⁱⁱ —Tl1—Se4 ^{vii}	53.678 (14)	Se1 ⁱⁱ —Se1—Se1 ^{xiii}	56.776 (11)
Tl1 ⁱⁱ —Tl1—Se4 ^v	125.76 (2)	Se1 ⁱⁱ —Se1—Se3 ^x	123.297 (17)
Tl1 ⁱⁱ —Tl1—Se4 ^{vi}	54.236 (14)	Se1 ⁱⁱ —Se1—Se3 ^{xi}	56.703 (11)
Tl1 ⁱⁱⁱ —Tl1—Se2 ^v	138.86 (2)	Se1 ^{xii} —Se1—Se1 ^{xiii}	66.448 (14)
Tl1 ⁱⁱⁱ —Tl1—Se2 ^{vi}	138.86 (2)	Se1 ^{xiii} —Se1—Se2	142.961 (13)

Tl1 ⁱⁱⁱ —Tl1—Se3 ⁱⁱⁱ	134.67 (5)	Se1 ^{xii} —Se1—Se3 ^x	81.396 (15)
Tl1 ⁱⁱⁱ —Tl1—Se4 ^{iv}	78.22 (4)	Se1 ^{xii} —Se1—Se3 ^{xi}	116.871 (19)
Tl1 ⁱⁱⁱ —Tl1—Se4 ^{vii}	78.22 (4)	Se1 ^{xiii} —Se1—Se2	142.961 (13)
Tl1 ⁱⁱⁱ —Tl1—Se4 ^v	75.00 (4)	Se1 ^{xiii} —Se1—Se3 ^x	116.871 (19)
Tl1 ⁱⁱⁱ —Tl1—Se4 ^{vi}	75.00 (4)	Se1 ^{xiii} —Se1—Se3 ^{xi}	81.396 (15)
Tl2 ^{iv} —Tl1—Se2 ^v	138.86 (3)	Se2—Se1—Se3 ^x	65.381 (17)
Tl2 ^{iv} —Tl1—Se2 ^{vi}	138.86 (3)	Se2—Se1—Se3 ^{xi}	65.381 (17)
Tl2 ^{iv} —Tl1—Se3 ⁱⁱⁱ	134.67 (7)	Se3 ^x —Se1—Se3 ^{xi}	66.594 (15)
Tl2 ^{iv} —Tl1—Se4 ^{iv}	78.22 (5)	Tl1 ^v —Se2—Tl1 ^{vi}	76.10 (2)
Tl2 ^{iv} —Tl1—Se4 ^{vii}	78.22 (5)	Tl1 ^v —Se2—Tl2 ⁱ	7.689 (13)
Tl2 ^{iv} —Tl1—Se4 ^v	75.00 (5)	Tl1 ^v —Se2—Tl2	69.244 (19)
Tl2 ^{iv} —Tl1—Se4 ^{vi}	75.00 (5)	Tl1 ^v —Se2—In2	124.82 (2)
Se2 ^v —Tl1—Se2 ^{vi}	76.10 (3)	Tl1 ^v —Se2—In2 ^v	87.489 (18)
Se2 ^v —Tl1—Se3 ⁱⁱⁱ	68.55 (2)	Tl1 ^v —Se2—In2 ^{vi}	148.67 (3)
Se2 ^v —Tl1—Se4 ^{iv}	88.171 (18)	Tl1 ^v —Se2—Se1	118.10 (2)
Se2 ^v —Tl1—Se4 ^{vii}	134.29 (3)	Tl1 ^v —Se2—Se2 ⁱ	51.949 (16)
Se2 ^v —Tl1—Se4 ^v	69.98 (2)	Tl1 ^v —Se2—Se2 ⁱⁱ	128.05 (2)
Se2 ^v —Tl1—Se4 ^{vi}	112.22 (3)	Tl1 ^v —Se2—Se2 ^v	110.899 (15)
Se2 ^{vi} —Tl1—Se3 ⁱⁱⁱ	68.55 (2)	Tl1 ^v —Se2—Se2 ^{vi}	168.61 (2)
Se2 ^{vi} —Tl1—Se4 ^{iv}	134.29 (3)	Tl1 ^v —Se2—Se3 ^x	61.888 (19)
Se2 ^{vi} —Tl1—Se4 ^{vii}	88.171 (18)	Tl1 ^v —Se2—Se3 ^{xi}	98.64 (2)
Se2 ^{vi} —Tl1—Se4 ^v	112.22 (3)	Tl1 ^v —Se2—Se4	57.184 (19)
Se2 ^{vi} —Tl1—Se4 ^{vi}	69.98 (2)	Tl1 ^{vi} —Se2—Tl2 ⁱ	69.244 (19)
Se3 ⁱⁱⁱ —Tl1—Se4 ^{iv}	65.75 (2)	Tl1 ^{vi} —Se2—Tl2	7.689 (13)
Se3 ⁱⁱⁱ —Tl1—Se4 ^{vii}	65.75 (2)	Tl1 ^{vi} —Se2—In2	124.82 (2)
Se3 ⁱⁱⁱ —Tl1—Se4 ^v	136.79 (2)	Tl1 ^{vi} —Se2—In2 ^v	148.67 (3)
Se3 ⁱⁱⁱ —Tl1—Se4 ^{vi}	136.79 (2)	Tl1 ^{vi} —Se2—In2 ^{vi}	87.489 (18)
Se4 ^{iv} —Tl1—Se4 ^{vii}	72.64 (2)	Tl1 ^{vi} —Se2—Se1	118.10 (2)
Se4 ^{iv} —Tl1—Se4 ^v	101.558 (16)	Tl1 ^{vi} —Se2—Se2 ⁱ	128.05 (2)
Se4 ^{iv} —Tl1—Se4 ^{vi}	153.22 (4)	Tl1 ^{vi} —Se2—Se2 ⁱⁱ	51.949 (16)
Se4 ^{vii} —Tl1—Se4 ^v	153.22 (4)	Tl1 ^{vi} —Se2—Se2 ^v	168.61 (2)
Se4 ^{vii} —Tl1—Se4 ^{vi}	101.558 (16)	Tl1 ^{vi} —Se2—Se2 ^{vi}	110.899 (15)
Se4 ^v —Tl1—Se4 ^{vi}	71.529 (19)	Tl1 ^{vi} —Se2—Se3 ^x	98.64 (2)
Tl1 ^{xi} —Tl2—Tl1 ^{vi}	180.0 (5)	Tl1 ^{vi} —Se2—Se3 ^{xi}	61.888 (19)
Tl1 ^{xi} —Tl2—Tl2 ⁱ	90	Tl1 ^{vi} —Se2—Se4	57.184 (19)
Tl1 ^{xi} —Tl2—Tl2 ⁱⁱ	90	Tl2 ⁱ —Se2—Tl2	62.186 (13)
Tl1 ^{xi} —Tl2—Se2	146.55 (2)	Tl2 ⁱ —Se2—In2	125.34 (2)
Tl1 ^{xi} —Tl2—Se2 ⁱⁱ	146.55 (2)	Tl2 ⁱ —Se2—In2 ^v	95.178 (13)
Tl1 ^{xi} —Tl2—Se2 ^{viii}	33.45 (2)	Tl2 ⁱ —Se2—In2 ^{vi}	147.42 (2)
Tl1 ^{xi} —Tl2—Se2 ^{ix}	33.45 (2)	Tl2 ⁱ —Se2—Se1	123.962 (15)
Tl1 ^{xi} —Tl2—Se4	88.30 (5)	Tl2 ⁱ —Se2—Se2 ⁱ	58.907 (12)
Tl1 ^{xi} —Tl2—Se4 ⁱⁱ	88.30 (5)	Tl2 ⁱ —Se2—Se2 ⁱⁱ	121.093 (19)
Tl1 ^{xi} —Tl2—Se4 ^{viii}	91.70 (5)	Tl2 ⁱ —Se2—Se2 ^v	117.058 (10)
Tl1 ^{xi} —Tl2—Se4 ^{ix}	91.70 (5)	Tl2 ⁱ —Se2—Se2 ^{vi}	167.79 (2)
Tl1 ^{vi} —Tl2—Tl2 ⁱ	90	Tl2 ⁱ —Se2—Se3 ^x	67.384 (13)
Tl1 ^{vi} —Tl2—Tl2 ⁱⁱ	90	Tl2 ⁱ —Se2—Se3 ^{xi}	97.822 (17)
Tl1 ^{vi} —Tl2—Se2	33.45 (2)	Tl2 ⁱ —Se2—Se4	50.873 (12)
Tl1 ^{vi} —Tl2—Se2 ⁱⁱ	33.45 (2)	Tl2—Se2—In2	125.34 (2)

Tl1 ^{vi} —Tl2—Se2 ^{viii}	146.55 (2)	Tl2—Se2—In2 ^v	147.42 (2)
Tl1 ^{vi} —Tl2—Se2 ^{ix}	146.55 (2)	Tl2—Se2—In2 ^{vi}	95.178 (13)
Tl1 ^{vi} —Tl2—Se4	91.70 (5)	Tl2—Se2—Se1	123.962 (15)
Tl1 ^{vi} —Tl2—Se4 ⁱⁱ	91.70 (5)	Tl2—Se2—Se2 ⁱ	121.093 (19)
Tl1 ^{vi} —Tl2—Se4 ^{viii}	88.30 (5)	Tl2—Se2—Se2 ⁱⁱ	58.907 (12)
Tl1 ^{vi} —Tl2—Se4 ^{ix}	88.30 (5)	Tl2—Se2—Se2 ^v	167.79 (2)
Tl2 ⁱ —Tl2—Tl2 ⁱⁱ	180.0 (5)	Tl2—Se2—Se2 ^{vi}	117.058 (10)
Tl2 ⁱ —Tl2—Se2	58.907 (6)	Tl2—Se2—Se3 ^x	97.822 (17)
Tl2 ⁱ —Tl2—Se2 ⁱⁱ	121.093 (6)	Tl2—Se2—Se3 ^{xi}	67.384 (13)
Tl2 ⁱ —Tl2—Se2 ^{viii}	58.907 (6)	Tl2—Se2—Se4	50.873 (12)
Tl2 ⁱ —Tl2—Se2 ^{ix}	121.093 (6)	In2—Se2—In2 ^v	86.47 (2)
Tl2 ⁱ —Tl2—Se4	52.785 (7)	In2—Se2—In2 ^{vi}	86.47 (2)
Tl2 ⁱ —Tl2—Se4 ⁱⁱ	127.215 (7)	In2—Se2—Se1	96.79 (3)
Tl2 ⁱ —Tl2—Se4 ^{viii}	52.785 (7)	In2—Se2—Se2 ^v	43.875 (14)
Tl2 ⁱ —Tl2—Se4 ^{ix}	127.215 (7)	In2—Se2—Se2 ^{vi}	43.875 (14)
Tl2 ⁱⁱ —Tl2—Se2	121.093 (6)	In2—Se2—Se3 ^x	136.53 (2)
Tl2 ⁱⁱ —Tl2—Se2 ⁱⁱ	58.907 (6)	In2—Se2—Se3 ^{xi}	136.53 (2)
Tl2 ⁱⁱ —Tl2—Se2 ^{viii}	121.093 (6)	In2—Se2—Se4	89.96 (2)
Tl2 ⁱⁱ —Tl2—Se2 ^{ix}	58.907 (6)	In2 ^v —Se2—In2 ^{vi}	93.52 (3)
Tl2 ⁱⁱ —Tl2—Se4	127.215 (7)	In2 ^v —Se2—Se1	47.915 (14)
Tl2 ⁱⁱ —Tl2—Se4 ⁱⁱ	52.785 (7)	In2 ^v —Se2—Se2 ⁱ	43.241 (14)
Tl2 ⁱⁱ —Tl2—Se4 ^{viii}	127.215 (7)	In2 ^v —Se2—Se2 ⁱⁱ	136.76 (3)
Tl2 ⁱⁱ —Tl2—Se4 ^{ix}	52.785 (7)	In2 ^v —Se2—Se2 ^v	42.593 (15)
Se2—Tl2—Se2 ⁱⁱ	62.186 (10)	In2 ^v —Se2—Se2 ^{vi}	90.05 (2)
Se2—Tl2—Se2 ^{viii}	117.814 (10)	In2 ^v —Se2—Se3 ^x	50.066 (15)
Se2—Tl2—Se2 ^{ix}	180.0 (5)	In2 ^v —Se2—Se3 ^{xi}	95.31 (2)
Se2—Tl2—Se4	63.828 (16)	In2 ^v —Se2—Se4	133.020 (14)
Se2—Tl2—Se4 ⁱⁱ	100.580 (14)	In2 ^{vi} —Se2—Se1	47.915 (14)
Se2—Tl2—Se4 ^{viii}	79.420 (14)	In2 ^{vi} —Se2—Se2 ⁱ	136.76 (3)
Se2—Tl2—Se4 ^{ix}	116.172 (16)	In2 ^{vi} —Se2—Se2 ⁱⁱ	43.241 (14)
Se2 ⁱⁱ —Tl2—Se2 ^{viii}	180.0 (5)	In2 ^{vi} —Se2—Se2 ^v	90.05 (2)
Se2 ⁱⁱ —Tl2—Se2 ^{ix}	117.814 (10)	In2 ^{vi} —Se2—Se2 ^{vi}	42.593 (15)
Se2 ⁱⁱ —Tl2—Se4	100.580 (14)	In2 ^{vi} —Se2—Se3 ^x	95.31 (2)
Se2 ⁱⁱ —Tl2—Se4 ⁱⁱ	63.828 (16)	In2 ^{vi} —Se2—Se3 ^{xi}	50.066 (15)
Se2 ⁱⁱ —Tl2—Se4 ^{viii}	116.172 (16)	In2 ^{vi} —Se2—Se4	133.020 (14)
Se2 ⁱⁱ —Tl2—Se4 ^{ix}	79.420 (14)	Se1—Se2—Se2 ^v	67.339 (17)
Se2 ^{viii} —Tl2—Se2 ^{ix}	62.186 (10)	Se1—Se2—Se2 ^{vi}	67.339 (17)
Se2 ^{viii} —Tl2—Se4	79.420 (14)	Se1—Se2—Se3 ^x	56.591 (16)
Se2 ^{viii} —Tl2—Se4 ⁱⁱ	116.172 (16)	Se1—Se2—Se3 ^{xi}	56.591 (16)
Se2 ^{viii} —Tl2—Se4 ^{viii}	63.828 (16)	Se1—Se2—Se4	173.25 (2)
Se2 ^{viii} —Tl2—Se4 ^{ix}	100.580 (14)	Se2 ⁱ —Se2—Se2 ⁱⁱ	180.0 (5)
Se2 ^{ix} —Tl2—Se4	116.172 (16)	Se2 ⁱ —Se2—Se2 ^v	59.612 (13)
Se2 ^{ix} —Tl2—Se4 ⁱⁱ	79.420 (14)	Se2 ⁱ —Se2—Se2 ^{vi}	120.388 (19)
Se2 ^{ix} —Tl2—Se4 ^{viii}	100.580 (14)	Se2 ⁱ —Se2—Se3 ^x	59.729 (11)
Se2 ^{ix} —Tl2—Se4 ^{ix}	63.828 (16)	Se2 ⁱ —Se2—Se3 ^{xi}	120.271 (16)
Se4—Tl2—Se4 ⁱⁱ	74.429 (12)	Se2 ⁱⁱ —Se2—Se2 ^v	120.388 (19)
Se4—Tl2—Se4 ^{viii}	105.571 (12)	Se2 ⁱⁱ —Se2—Se2 ^{vi}	59.612 (13)
Se4—Tl2—Se4 ^{ix}	180.0 (5)	Se2 ⁱⁱ —Se2—Se3 ^x	120.271 (16)

Se4 ⁱⁱ —Tl2—Se4 ^{viii}	180.0 (5)	Se2 ⁱⁱ —Se2—Se3 ^{xi}	59.729 (11)
Se4 ⁱⁱ —Tl2—Se4 ^{ix}	105.571 (12)	Se2 ^v —Se2—Se2 ^{vi}	60.777 (14)
Se4 ^{viii} —Tl2—Se4 ^{ix}	74.429 (12)	Se2 ^v —Se2—Se3 ^x	92.659 (16)
In1 ⁱ —In1—In1 ⁱⁱ	180.0 (5)	Se2 ^v —Se2—Se3 ^{xi}	123.81 (2)
In1 ⁱ —In1—In3 ^x	57.447 (5)	Se2 ^v —Se2—Se4	118.249 (18)
In1 ⁱ —In1—In3 ^{xi}	122.553 (5)	Se2 ^{vi} —Se2—Se3 ^x	123.81 (2)
In1 ⁱ —In1—In3 ^{xii}	57.447 (5)	Se2 ^{vi} —Se2—Se3 ^{xi}	92.659 (16)
In1 ⁱ —In1—In3 ^{xiii}	122.553 (5)	Se2 ^{vi} —Se2—Se4	118.249 (18)
In1 ⁱ —In1—Se3 ^x	42.872 (10)	Se3 ^x —Se2—Se3 ^{xi}	60.542 (13)
In1 ⁱ —In1—Se3 ^{xi}	137.128 (10)	Se3 ^x —Se2—Se4	117.94 (2)
In1 ⁱ —In1—Se3 ^{xii}	42.872 (10)	Se3 ^{xi} —Se2—Se4	117.94 (2)
In1 ⁱ —In1—Se3 ^{xiii}	137.128 (10)	Tl1 ⁱⁱⁱ —Se3—In1 ^{iv}	97.18 (2)
In1 ⁱ —In1—Se4 ^{xiv}	90	Tl1 ⁱⁱⁱ —Se3—In1 ^{vii}	97.18 (2)
In1 ⁱ —In1—Se4 ^{viii}	90	Tl1 ⁱⁱⁱ —Se3—Cr ^{iv}	97.18 (2)
In1 ⁱⁱ —In1—Cr ⁱ	180.0 (5)	Tl1 ⁱⁱⁱ —Se3—Cr ^{vii}	97.18 (2)
In1 ⁱⁱ —In1—In3 ^x	122.553 (5)	Tl1 ⁱⁱⁱ —Se3—In2 ⁱⁱⁱ	74.45 (2)
In1 ⁱⁱ —In1—In3 ^{xi}	57.447 (5)	Tl1 ⁱⁱⁱ —Se3—In3 ^{xv}	172.46 (3)
In1 ⁱⁱ —In1—In3 ^{xii}	122.553 (5)	Tl1 ⁱⁱⁱ —Se3—Se1 ^{iv}	107.29 (2)
In1 ⁱⁱ —In1—In3 ^{xiii}	57.447 (5)	Tl1 ⁱⁱⁱ —Se3—Se1 ^{vii}	107.29 (2)
In1 ⁱⁱ —In1—Se3 ^x	137.128 (10)	Tl1 ⁱⁱⁱ —Se3—Se2 ^{iv}	49.567 (17)
In1 ⁱⁱ —In1—Se3 ^{xi}	42.872 (10)	Tl1 ⁱⁱⁱ —Se3—Se2 ^{vii}	49.567 (17)
In1 ⁱⁱ —In1—Se3 ^{xii}	137.128 (10)	Tl1 ⁱⁱⁱ —Se3—Se3 ^{xv}	100.59 (3)
In1 ⁱⁱ —In1—Se3 ^{xiii}	42.872 (10)	Tl1 ⁱⁱⁱ —Se3—Se4 ^{xvi}	141.961 (17)
In1 ⁱⁱ —In1—Se4 ^{xiv}	90	Tl1 ⁱⁱⁱ —Se3—Se4 ^{xvii}	141.961 (17)
In1 ⁱⁱ —In1—Se4 ^{viii}	90	Tl1 ⁱⁱⁱ —Se3—Se4 ^v	52.372 (17)
Cr ⁱ —In1—Cr ⁱⁱ	180.0 (5)	Tl1 ⁱⁱⁱ —Se3—Se4 ^{vi}	52.372 (17)
Cr ⁱ —In1—In3 ^x	57.447 (5)	In1 ^{iv} —Se3—In1 ^{vii}	94.256 (19)
Cr ⁱ —In1—In3 ^{xi}	122.553 (5)	In1 ^{iv} —Se3—Cr ^{vii}	94.256 (19)
Cr ⁱ —In1—In3 ^{xii}	57.447 (5)	In1 ^{iv} —Se3—In2 ⁱⁱⁱ	132.673 (10)
Cr ⁱ —In1—In3 ^{xiii}	122.553 (5)	In1 ^{iv} —Se3—In3 ^{xv}	87.929 (17)
Cr ⁱ —In1—Se3 ^x	42.872 (10)	In1 ^{iv} —Se3—Se1 ^{iv}	94.758 (12)
Cr ⁱ —In1—Se3 ^{xi}	137.128 (10)	In1 ^{iv} —Se3—Se1 ^{vii}	152.58 (2)
Cr ⁱ —In1—Se3 ^{xii}	42.872 (10)	In1 ^{iv} —Se3—Se2 ^{iv}	95.340 (12)
Cr ⁱ —In1—Se3 ^{xiii}	137.128 (10)	In1 ^{iv} —Se3—Se2 ^{vii}	146.30 (2)
Cr ⁱⁱ —In1—In3 ^x	122.553 (5)	In1 ^{iv} —Se3—Se3 ⁱ	42.872 (9)
Cr ⁱⁱ —In1—In3 ^{xi}	57.447 (5)	In1 ^{iv} —Se3—Se3 ⁱⁱ	137.128 (19)
Cr ⁱⁱ —In1—In3 ^{xii}	122.553 (5)	In1 ^{iv} —Se3—Se3 ^{xv}	47.128 (10)
Cr ⁱⁱ —In1—In3 ^{xiii}	57.447 (5)	In1 ^{iv} —Se3—Se4 ^{xvi}	45.411 (12)
Cr ⁱⁱ —In1—Se3 ^x	137.128 (10)	In1 ^{iv} —Se3—Se4 ^{xvii}	93.072 (18)
Cr ⁱⁱ —In1—Se3 ^{xi}	42.872 (10)	In1 ^{iv} —Se3—Se4 ^v	45.298 (13)
Cr ⁱⁱ —In1—Se3 ^{xii}	137.128 (10)	In1 ^{iv} —Se3—Se4 ^{vi}	92.907 (19)
Cr ⁱⁱ —In1—Se3 ^{xiii}	42.872 (10)	In1 ^{vii} —Se3—Cr ^{iv}	94.256 (19)
In3 ^x —In1—In3 ^{xi}	65.105 (9)	In1 ^{vii} —Se3—Cr ^{vii}	0.0 (5)
In3 ^x —In1—In3 ^{xii}	114.895 (9)	In1 ^{vii} —Se3—In2 ⁱⁱⁱ	132.673 (10)
In3 ^x —In1—In3 ^{xiii}	180.0 (5)	In1 ^{vii} —Se3—In3 ^{xv}	87.929 (17)
In3 ^x —In1—Se3 ^x	85.411 (15)	In1 ^{vii} —Se3—Se1 ^{iv}	152.58 (2)
In3 ^x —In1—Se3 ^{xi}	135.128 (16)	In1 ^{vii} —Se3—Se1 ^{vii}	94.758 (12)
In3 ^x —In1—Se3 ^{xii}	44.872 (16)	In1 ^{vii} —Se3—Se2 ^{iv}	146.30 (2)

In3 ^x —In1—Se3 ^{xiii}	94.589 (15)	In1 ^{vii} —Se3—Se2 ^{vii}	95.340 (12)
In3 ^x —In1—Se4 ^{xiv}	134.936 (11)	In1 ^{vii} —Se3—Se3 ⁱ	137.128 (19)
In3 ^x —In1—Se4 ^{viii}	45.064 (11)	In1 ^{vii} —Se3—Se3 ⁱⁱ	42.872 (9)
In3 ^{xi} —In1—In3 ^{xii}	180.0 (5)	In1 ^{vii} —Se3—Se3 ^{xv}	47.128 (10)
In3 ^{xi} —In1—In3 ^{xiii}	114.895 (9)	In1 ^{vii} —Se3—Se4 ^{xvi}	93.072 (18)
In3 ^{xi} —In1—Se3 ^x	135.128 (16)	In1 ^{vii} —Se3—Se4 ^{xvii}	45.411 (12)
In3 ^{xi} —In1—Se3 ^{xi}	85.411 (15)	In1 ^{vii} —Se3—Se4 ^v	92.907 (19)
In3 ^{xi} —In1—Se3 ^{xii}	94.589 (15)	In1 ^{vii} —Se3—Se4 ^{vi}	45.298 (13)
In3 ^{xi} —In1—Se3 ^{xiii}	44.872 (16)	Cr ^{iv} —Se3—Cr ^{vii}	94.256 (19)
In3 ^{xi} —In1—Se4 ^{xiv}	134.936 (11)	Cr ^{iv} —Se3—In2 ⁱⁱⁱ	132.673 (10)
In3 ^{xi} —In1—Se4 ^{viii}	45.064 (11)	Cr ^{iv} —Se3—In3 ^{xv}	87.929 (17)
In3 ^{xii} —In1—In3 ^{xiii}	65.105 (9)	Cr ^{iv} —Se3—Se1 ^{iv}	94.758 (12)
In3 ^{xii} —In1—Se3 ^x	44.872 (16)	Cr ^{iv} —Se3—Se1 ^{vii}	152.58 (2)
In3 ^{xii} —In1—Se3 ^{xi}	94.589 (15)	Cr ^{iv} —Se3—Se2 ^{iv}	95.340 (12)
In3 ^{xii} —In1—Se3 ^{xii}	85.411 (15)	Cr ^{iv} —Se3—Se2 ^{vii}	146.30 (2)
In3 ^{xii} —In1—Se3 ^{xiii}	135.128 (16)	Cr ^{iv} —Se3—Se3 ⁱ	42.872 (9)
In3 ^{xii} —In1—Se4 ^{xiv}	45.064 (11)	Cr ^{iv} —Se3—Se3 ⁱⁱ	137.128 (19)
In3 ^{xii} —In1—Se4 ^{viii}	134.936 (11)	Cr ^{iv} —Se3—Se3 ^{xv}	47.128 (10)
In3 ^{xiii} —In1—Se3 ^x	94.589 (15)	Cr ^{iv} —Se3—Se4 ^{xvi}	45.411 (12)
In3 ^{xiii} —In1—Se3 ^{xi}	44.872 (16)	Cr ^{iv} —Se3—Se4 ^{xvii}	93.072 (18)
In3 ^{xiii} —In1—Se3 ^{xii}	135.128 (16)	Cr ^{iv} —Se3—Se4 ^v	45.298 (13)
In3 ^{xiii} —In1—Se3 ^{xiii}	85.411 (15)	Cr ^{iv} —Se3—Se4 ^{vi}	92.907 (19)
In3 ^{xiii} —In1—Se4 ^{xiv}	45.064 (11)	Cr ^{vii} —Se3—In2 ⁱⁱⁱ	132.673 (10)
In3 ^{xiii} —In1—Se4 ^{viii}	134.936 (11)	Cr ^{vii} —Se3—In3 ^{xv}	87.929 (17)
Se3 ^x —In1—Se3 ^{xi}	94.256 (15)	Cr ^{vii} —Se3—Se1 ^{iv}	152.58 (2)
Se3 ^x —In1—Se3 ^{xii}	85.744 (15)	Cr ^{vii} —Se3—Se1 ^{vii}	94.758 (12)
Se3 ^x —In1—Se3 ^{xiii}	180.0 (5)	Cr ^{vii} —Se3—Se2 ^{iv}	146.30 (2)
Se3 ^x —In1—Se4 ^{xiv}	89.889 (17)	Cr ^{vii} —Se3—Se2 ^{vii}	95.340 (12)
Se3 ^x —In1—Se4 ^{viii}	90.111 (17)	Cr ^{vii} —Se3—Se3 ⁱ	137.128 (19)
Se3 ^{xi} —In1—Se3 ^{xii}	180.0 (5)	Cr ^{vii} —Se3—Se3 ⁱⁱ	42.872 (9)
Se3 ^{xi} —In1—Se3 ^{xiii}	85.744 (15)	Cr ^{vii} —Se3—Se3 ^{xv}	47.128 (10)
Se3 ^{xi} —In1—Se4 ^{xiv}	89.889 (17)	Cr ^{vii} —Se3—Se4 ^{xvi}	93.072 (18)
Se3 ^{xi} —In1—Se4 ^{viii}	90.111 (17)	Cr ^{vii} —Se3—Se4 ^{xvii}	45.411 (12)
Se3 ^{xii} —In1—Se3 ^{xiii}	94.256 (15)	Cr ^{vii} —Se3—Se4 ^v	92.907 (19)
Se3 ^{xii} —In1—Se4 ^{xiv}	90.111 (17)	Cr ^{vii} —Se3—Se4 ^{vi}	45.298 (13)
Se3 ^{xii} —In1—Se4 ^{viii}	89.889 (17)	In2 ⁱⁱⁱ —Se3—In3 ^{xv}	98.01 (3)
Se3 ^{xiii} —In1—Se4 ^{xiv}	90.111 (17)	In2 ⁱⁱⁱ —Se3—Se1 ^{iv}	47.708 (13)
Se3 ^{xiii} —In1—Se4 ^{viii}	89.889 (17)	In2 ⁱⁱⁱ —Se3—Se1 ^{vii}	47.708 (13)
In1 ⁱ —Cr—In3 ^x	57.447 (5)	In2 ⁱⁱⁱ —Se3—Se2 ^{iv}	43.670 (13)
In1 ⁱ —Cr—In3 ^{xi}	122.553 (5)	In2 ⁱⁱⁱ —Se3—Se2 ^{vii}	43.670 (13)
In1 ⁱ —Cr—In3 ^{xii}	57.447 (5)	In2 ⁱⁱⁱ —Se3—Se3 ⁱ	90.000 (11)
In1 ⁱ —Cr—In3 ^{xiii}	122.553 (5)	In2 ⁱⁱⁱ —Se3—Se3 ⁱⁱ	90.000 (11)
In1 ⁱ —Cr—Se3 ^x	42.872 (10)	In2 ⁱⁱⁱ —Se3—Se3 ^{xv}	175.04 (3)
In1 ⁱ —Cr—Se3 ^{xi}	137.128 (10)	In2 ⁱⁱⁱ —Se3—Se4 ^{xvi}	122.44 (2)
In1 ⁱ —Cr—Se3 ^{xii}	42.872 (10)	In2 ⁱⁱⁱ —Se3—Se4 ^{xvii}	122.44 (2)
In1 ⁱ —Cr—Se3 ^{xiii}	137.128 (10)	In2 ⁱⁱⁱ —Se3—Se4 ^v	114.61 (2)
In1 ⁱⁱ —Cr—In3 ^x	122.553 (5)	In2 ⁱⁱⁱ —Se3—Se4 ^{vi}	114.61 (2)
In1 ⁱⁱ —Cr—In3 ^{xi}	57.447 (5)	In3 ^{xv} —Se3—Se1 ^{iv}	66.595 (18)

In1 ⁱⁱ —Cr—In3 ^{xii}	122.553 (5)	In3 ^{xv} —Se3—Se1 ^{vii}	66.595 (18)
In1 ⁱⁱ —Cr—In3 ^{xiii}	57.447 (5)	In3 ^{xv} —Se3—Se2 ^{iv}	124.62 (2)
In1 ⁱⁱ —Cr—Se3 ^x	137.128 (10)	In3 ^{xv} —Se3—Se2 ^{vii}	124.62 (2)
In1 ⁱⁱ —Cr—Se3 ^{xi}	42.872 (10)	In3 ^{xv} —Se3—Se3 ⁱ	90.000 (14)
In1 ⁱⁱ —Cr—Se3 ^{xii}	137.128 (10)	In3 ^{xv} —Se3—Se3 ⁱⁱ	90.000 (14)
In1 ⁱⁱ —Cr—Se3 ^{xiii}	42.872 (10)	In3 ^{xv} —Se3—Se3 ^{xv}	86.96 (2)
Cr ⁱ —Cr—Cr ⁱⁱ	180.0 (5)	In3 ^{xv} —Se3—Se4 ^{xvi}	42.569 (14)
Cr ⁱ —Cr—In3 ^x	57.447 (5)	In3 ^{xv} —Se3—Se4 ^{xvii}	42.569 (14)
Cr ⁱ —Cr—In3 ^{xi}	122.553 (5)	In3 ^{xv} —Se3—Se4 ^v	133.180 (18)
Cr ⁱ —Cr—In3 ^{xii}	57.447 (5)	In3 ^{xv} —Se3—Se4 ^{vi}	133.180 (18)
Cr ⁱ —Cr—In3 ^{xiii}	122.553 (5)	Se1 ^{iv} —Se3—Se1 ^{vii}	66.594 (15)
Cr ⁱ —Cr—Se3 ^x	42.872 (10)	Se1 ^{iv} —Se3—Se2 ^{iv}	58.029 (16)
Cr ⁱ —Cr—Se3 ^{xi}	137.128 (10)	Se1 ^{iv} —Se3—Se2 ^{vii}	91.374 (18)
Cr ⁱ —Cr—Se3 ^{xii}	42.872 (10)	Se1 ^{iv} —Se3—Se3 ⁱ	56.703 (12)
Cr ⁱ —Cr—Se3 ^{xiii}	137.128 (10)	Se1 ^{iv} —Se3—Se3 ⁱⁱ	123.297 (18)
Cr ⁱⁱ —Cr—In3 ^x	122.553 (5)	Se1 ^{iv} —Se3—Se3 ^{xv}	135.502 (16)
Cr ⁱⁱ —Cr—In3 ^{xi}	57.447 (5)	Se1 ^{iv} —Se3—Se4 ^{xvi}	75.321 (16)
Cr ⁱⁱ —Cr—In3 ^{xii}	122.553 (5)	Se1 ^{iv} —Se3—Se4 ^{xvii}	108.22 (2)
Cr ⁱⁱ —Cr—In3 ^{xiii}	57.447 (5)	Se1 ^{iv} —Se3—Se4 ^v	111.678 (12)
Cr ⁱⁱ —Cr—Se3 ^x	137.128 (10)	Se1 ^{iv} —Se3—Se4 ^{vi}	159.11 (2)
Cr ⁱⁱ —Cr—Se3 ^{xi}	42.872 (10)	Se1 ^{vii} —Se3—Se2 ^{iv}	91.374 (18)
Cr ⁱⁱ —Cr—Se3 ^{xii}	137.128 (10)	Se1 ^{vii} —Se3—Se2 ^{vii}	58.029 (16)
Cr ⁱⁱ —Cr—Se3 ^{xiii}	42.872 (10)	Se1 ^{vii} —Se3—Se3 ⁱ	123.297 (18)
In3 ^x —Cr—In3 ^{xi}	65.105 (9)	Se1 ^{vii} —Se3—Se3 ⁱⁱ	56.703 (12)
In3 ^x —Cr—In3 ^{xii}	114.895 (9)	Se1 ^{vii} —Se3—Se3 ^{xv}	135.502 (16)
In3 ^x —Cr—In3 ^{xiii}	180.0 (5)	Se1 ^{vii} —Se3—Se4 ^{xvi}	108.22 (2)
In3 ^x —Cr—Se3 ^x	85.411 (15)	Se1 ^{vii} —Se3—Se4 ^{xvii}	75.321 (16)
In3 ^x —Cr—Se3 ^{xi}	135.128 (16)	Se1 ^{vii} —Se3—Se4 ^v	159.11 (2)
In3 ^x —Cr—Se3 ^{xii}	44.872 (16)	Se1 ^{vii} —Se3—Se4 ^{vi}	111.678 (12)
In3 ^x —Cr—Se3 ^{xiii}	94.589 (15)	Se2 ^{iv} —Se3—Se2 ^{vii}	60.542 (13)
In3 ^x —Cr—Se4 ^{xiv}	134.936 (11)	Se2 ^{iv} —Se3—Se3 ⁱ	59.729 (11)
In3 ^x —Cr—Se4 ^{xviii}	45.064 (11)	Se2 ^{iv} —Se3—Se3 ⁱⁱ	120.271 (16)
In3 ^{xi} —Cr—In3 ^{xii}	180.0 (5)	Se2 ^{iv} —Se3—Se3 ^{xv}	132.827 (19)
In3 ^{xi} —Cr—In3 ^{xiii}	114.895 (9)	Se2 ^{iv} —Se3—Se4 ^{xvi}	116.325 (11)
In3 ^{xi} —Cr—Se3 ^x	135.128 (16)	Se2 ^{iv} —Se3—Se4 ^{xvii}	164.40 (2)
In3 ^{xi} —Cr—Se3 ^{xi}	85.411 (15)	Se2 ^{iv} —Se3—Se4 ^v	71.825 (16)
In3 ^{xi} —Cr—Se3 ^{xii}	94.589 (15)	Se2 ^{iv} —Se3—Se4 ^{vi}	101.93 (2)
In3 ^{xi} —Cr—Se3 ^{xiii}	44.872 (16)	Se2 ^{vii} —Se3—Se3 ⁱ	120.271 (16)
In3 ^{xi} —Cr—Se4 ^{xiv}	134.936 (11)	Se2 ^{vii} —Se3—Se3 ⁱⁱ	59.729 (11)
In3 ^{xi} —Cr—Se4 ^{xviii}	45.064 (11)	Se2 ^{vii} —Se3—Se3 ^{xv}	132.827 (19)
In3 ^{xii} —Cr—In3 ^{xiii}	65.105 (9)	Se2 ^{vii} —Se3—Se4 ^{xvi}	164.40 (2)
In3 ^{xii} —Cr—Se3 ^x	44.872 (16)	Se2 ^{vii} —Se3—Se4 ^{xvii}	116.325 (11)
In3 ^{xii} —Cr—Se3 ^{xi}	94.589 (15)	Se2 ^{vii} —Se3—Se4 ^v	101.93 (2)
In3 ^{xii} —Cr—Se3 ^{xii}	85.411 (15)	Se2 ^{vii} —Se3—Se4 ^{vi}	71.825 (16)
In3 ^{xii} —Cr—Se3 ^{xiii}	135.128 (16)	Se3 ⁱ —Se3—Se3 ⁱⁱ	180.0 (5)
In3 ^{xii} —Cr—Se4 ^{xiv}	45.064 (11)	Se3 ⁱ —Se3—Se3 ^{xv}	90.000 (12)
In3 ^{xii} —Cr—Se4 ^{xviii}	134.936 (11)	Se3 ⁱ —Se3—Se4 ^{xvi}	58.969 (11)
In3 ^{xiii} —Cr—Se3 ^x	94.589 (15)	Se3 ⁱ —Se3—Se4 ^{xvii}	121.031 (17)

In3 ^{xiii} —Cr—Se3 ^{xi}	44.872 (16)	Se3 ⁱ —Se3—Se4 ^v	59.036 (12)
In3 ^{xiii} —Cr—Se3 ^{xii}	135.128 (16)	Se3 ⁱ —Se3—Se4 ^{vi}	120.964 (19)
In3 ^{xiii} —Cr—Se3 ^{xiii}	85.411 (15)	Se3 ⁱⁱ —Se3—Se3 ^{xv}	90.000 (12)
In3 ^{xiii} —Cr—Se4 ^{xiv}	45.064 (11)	Se3 ⁱⁱ —Se3—Se4 ^{xvi}	121.031 (17)
In3 ^{xiii} —Cr—Se4 ^{xviii}	134.936 (11)	Se3 ⁱⁱ —Se3—Se4 ^{xvii}	58.969 (11)
Se3 ^x —Cr—Se3 ^{xi}	94.256 (15)	Se3 ⁱⁱ —Se3—Se4 ^v	120.964 (19)
Se3 ^x —Cr—Se3 ^{xii}	85.744 (15)	Se3 ⁱⁱ —Se3—Se4 ^{vi}	59.036 (12)
Se3 ^x —Cr—Se3 ^{xiii}	180.0 (5)	Se3 ^{xv} —Se3—Se4 ^{xvi}	61.541 (16)
Se3 ^x —Cr—Se4 ^{xiv}	89.889 (17)	Se3 ^{xv} —Se3—Se4 ^{xvii}	61.541 (16)
Se3 ^x —Cr—Se4 ^{xviii}	90.111 (17)	Se3 ^{xv} —Se3—Se4 ^v	61.336 (16)
Se3 ^{xi} —Cr—Se3 ^{xii}	180.0 (5)	Se3 ^{xv} —Se3—Se4 ^{vi}	61.336 (16)
Se3 ^{xi} —Cr—Se3 ^{xiii}	85.744 (15)	Se4 ^{xvi} —Se3—Se4 ^{xvii}	62.063 (14)
Se3 ^{xi} —Cr—Se4 ^{xiv}	89.889 (17)	Se4 ^{xvi} —Se3—Se4 ^v	90.709 (15)
Se3 ^{xi} —Cr—Se4 ^{xviii}	90.111 (17)	Se4 ^{xvi} —Se3—Se4 ^{vi}	122.88 (2)
Se3 ^{xii} —Cr—Se3 ^{xiii}	94.256 (15)	Se4 ^{xvii} —Se3—Se4 ^v	122.88 (2)
Se3 ^{xii} —Cr—Se4 ^{xiv}	90.111 (17)	Se4 ^{xvii} —Se3—Se4 ^{vi}	90.709 (15)
Se3 ^{xii} —Cr—Se4 ^{xviii}	89.889 (17)	Se4 ^v —Se3—Se4 ^{vi}	61.929 (14)
Se3 ^{xiii} —Cr—Se4 ^{xiv}	90.111 (17)	Tl1 ^x —Se4—Tl1 ^{xi}	72.644 (18)
Se3 ^{xiii} —Cr—Se4 ^{xviii}	89.889 (17)	Tl1 ^x —Se4—Tl1 ^v	26.78 (3)
In2 ⁱ —In2—In2 ^v	57.450 (8)	Tl1 ^x —Se4—Tl1 ^{vi}	78.44 (2)
In2 ⁱ —In2—In2 ^{vi}	122.550 (12)	Tl1 ^x —Se4—Tl2 ⁱ	13.482 (18)
In2 ⁱ —In2—Se1 ^v	43.568 (12)	Tl1 ^x —Se4—Tl2	75.169 (16)
In2 ⁱ —In2—Se1 ^{vi}	136.432 (19)	Tl1 ^x —Se4—In1 ^{xviii}	105.91 (3)
In2 ⁱ —In2—Se2 ^v	43.241 (14)	Tl1 ^x —Se4—Cr ^{xviii}	105.91 (3)
In2 ⁱ —In2—Se2 ^{vi}	136.76 (2)	Tl1 ^x —Se4—In3 ^v	93.230 (15)
In2 ⁱ —In2—Se3 ⁱⁱⁱ	90.000 (9)	Tl1 ^x —Se4—In3 ^{vi}	162.86 (3)
In2 ⁱⁱ —In2—In2 ^v	122.550 (12)	Tl1 ^x —Se4—Se2	78.09 (2)
In2 ⁱⁱ —In2—In2 ^{vi}	57.450 (8)	Tl1 ^x —Se4—Se3 ^{xix}	104.602 (16)
In2 ⁱⁱ —In2—Se1 ^v	136.432 (19)	Tl1 ^x —Se4—Se3 ^{xx}	149.63 (3)
In2 ⁱⁱ —In2—Se1 ^{vi}	43.568 (12)	Tl1 ^x —Se4—Se3 ^v	61.88 (2)
In2 ⁱⁱ —In2—Se2 ^v	136.76 (2)	Tl1 ^x —Se4—Se3 ^{vi}	97.94 (2)
In2 ⁱⁱ —In2—Se2 ^{vi}	43.241 (14)	Tl1 ^x —Se4—Se4 ⁱ	53.678 (12)
In2 ^v —In2—In2 ^{vi}	65.100 (11)	Tl1 ^x —Se4—Se4 ⁱⁱ	126.322 (19)
In2 ^v —In2—Se1 ^v	95.040 (13)	Tl1 ^{xi} —Se4—Tl1 ^v	78.44 (2)
In2 ^v —In2—Se1 ^{vi}	150.17 (2)	Tl1 ^{xi} —Se4—Tl1 ^{vi}	26.78 (3)
In2 ^v —In2—Se2	47.491 (14)	Tl1 ^{xi} —Se4—Tl2 ⁱ	75.169 (16)
In2 ^v —In2—Se2 ^v	46.041 (16)	Tl1 ^{xi} —Se4—Tl2	13.482 (18)
In2 ^v —In2—Se2 ^{vi}	95.149 (19)	Tl1 ^{xi} —Se4—In1 ^{xviii}	105.91 (3)
In2 ^v —In2—Se3 ⁱⁱⁱ	132.304 (17)	Tl1 ^{xi} —Se4—Cr ^{xviii}	105.91 (3)
In2 ^{vi} —In2—Se1 ^v	150.17 (2)	Tl1 ^{xi} —Se4—In3 ^v	162.86 (3)
In2 ^{vi} —In2—Se1 ^{vi}	95.040 (13)	Tl1 ^{xi} —Se4—In3 ^{vi}	93.230 (15)
In2 ^{vi} —In2—Se2	47.491 (14)	Tl1 ^{xi} —Se4—Se2	78.09 (2)
In2 ^{vi} —In2—Se2 ^v	95.149 (19)	Tl1 ^{xi} —Se4—Se3 ^{xix}	149.63 (3)
In2 ^{vi} —In2—Se2 ^{vi}	46.041 (16)	Tl1 ^{xi} —Se4—Se3 ^{xx}	104.602 (16)
In2 ^{vi} —In2—Se3 ⁱⁱⁱ	132.304 (17)	Tl1 ^{xi} —Se4—Se3 ^v	97.94 (2)
Se1 ^v —In2—Se1 ^{vi}	92.86 (2)	Tl1 ^{xi} —Se4—Se3 ^{vi}	61.88 (2)
Se1 ^v —In2—Se2	102.70 (2)	Tl1 ^{xi} —Se4—Se4 ⁱ	126.322 (19)
Se1 ^v —In2—Se2 ^v	84.510 (16)	Tl1 ^{xi} —Se4—Se4 ⁱⁱ	53.678 (12)

Se1 ^v —In2—Se2 ^{vi}	163.74 (3)	Tl1 ^v —Se4—Tl1 ^{vi}	71.529 (18)
Se1 ^v —In2—Se3 ⁱⁱⁱ	77.503 (18)	Tl1 ^v —Se4—Tl2 ⁱ	13.300 (18)
Se1 ^{vi} —In2—Se2	102.70 (2)	Tl1 ^v —Se4—Tl2	74.560 (17)
Se1 ^{vi} —In2—Se2 ^v	163.74 (3)	Tl1 ^v —Se4—In1 ^{xviii}	130.51 (2)
Se1 ^{vi} —In2—Se2 ^{vi}	84.510 (16)	Tl1 ^v —Se4—Cr ^{xviii}	130.51 (2)
Se1 ^{vi} —In2—Se3 ⁱⁱⁱ	77.503 (18)	Tl1 ^v —Se4—In3 ^v	84.600 (17)
Se2—In2—Se2 ^v	93.53 (2)	Tl1 ^v —Se4—In3 ^{vi}	142.48 (3)
Se2—In2—Se2 ^{vi}	93.53 (2)	Tl1 ^v —Se4—Se2	52.84 (2)
Se2—In2—Se3 ⁱⁱⁱ	179.70 (3)	Tl1 ^v —Se4—Se3 ^{xix}	113.150 (12)
Se2 ^v —In2—Se2 ^{vi}	93.52 (2)	Tl1 ^v —Se4—Se3 ^{xx}	174.69 (2)
Se2 ^v —In2—Se3 ⁱⁱⁱ	86.26 (2)	Tl1 ^v —Se4—Se3 ^v	85.96 (2)
Se2 ^{vi} —In2—Se3 ⁱⁱⁱ	86.26 (2)	Tl1 ^v —Se4—Se3 ^{vi}	122.07 (3)
In1 ^{iv} —In3—In1 ^{vii}	65.105 (11)	Tl1 ^v —Se4—Se4 ⁱ	54.236 (13)
In1 ^{iv} —In3—Cr ^{iv}	0.0 (5)	Tl1 ^v —Se4—Se4 ⁱⁱ	125.764 (19)
In1 ^{iv} —In3—Cr ^{vii}	65.105 (11)	Tl1 ^{vi} —Se4—Tl2 ⁱ	74.560 (17)
In1 ^{iv} —In3—In3 ⁱ	57.447 (8)	Tl1 ^{vi} —Se4—Tl2	13.300 (18)
In1 ^{iv} —In3—In3 ⁱⁱ	122.553 (14)	Tl1 ^{vi} —Se4—In1 ^{xviii}	130.51 (2)
In1 ^{iv} —In3—Se1	146.097 (7)	Tl1 ^{vi} —Se4—Cr ^{xviii}	130.51 (2)
In1 ^{iv} —In3—Se1 ^{xii}	81.246 (13)	Tl1 ^{vi} —Se4—In3 ^v	142.48 (3)
In1 ^{iv} —In3—Se1 ^{xiii}	117.067 (18)	Tl1 ^{vi} —Se4—In3 ^{vi}	84.600 (17)
In1 ^{iv} —In3—Se3 ^{xv}	47.199 (12)	Tl1 ^{vi} —Se4—Se2	52.84 (2)
In1 ^{iv} —In3—Se4 ^v	47.930 (17)	Tl1 ^{vi} —Se4—Se3 ^{xix}	174.69 (2)
In1 ^{iv} —In3—Se4 ^{vi}	98.44 (2)	Tl1 ^{vi} —Se4—Se3 ^{xx}	113.150 (12)
In1 ^{vii} —In3—Cr ^{iv}	65.105 (11)	Tl1 ^{vi} —Se4—Se3 ^v	122.07 (3)
In1 ^{vii} —In3—Cr ^{vii}	0.0 (5)	Tl1 ^{vi} —Se4—Se3 ^{vi}	85.96 (2)
In1 ^{vii} —In3—In3 ⁱ	122.553 (14)	Tl1 ^{vi} —Se4—Se4 ⁱ	125.764 (19)
In1 ^{vii} —In3—In3 ⁱⁱ	57.447 (8)	Tl1 ^{vi} —Se4—Se4 ⁱⁱ	54.236 (13)
In1 ^{vii} —In3—Se1	146.097 (7)	Tl2 ⁱ —Se4—Tl2	74.429 (15)
In1 ^{vii} —In3—Se1 ^{xii}	117.067 (18)	Tl2 ⁱ —Se4—In1 ^{xviii}	118.427 (18)
In1 ^{vii} —In3—Se1 ^{xiii}	81.246 (13)	Tl2 ⁱ —Se4—Cr ^{xviii}	118.427 (18)
In1 ^{vii} —In3—Se3 ^{xv}	47.199 (12)	Tl2 ⁱ —Se4—In3 ^v	88.858 (13)
In1 ^{vii} —In3—Se4 ^v	98.44 (2)	Tl2 ⁱ —Se4—In3 ^{vi}	153.93 (3)
In1 ^{vii} —In3—Se4 ^{vi}	47.930 (17)	Tl2 ⁱ —Se4—Se2	65.299 (14)
Cr ^{iv} —In3—Cr ^{vii}	65.105 (11)	Tl2 ⁱ —Se4—Se3 ^{xix}	109.398 (10)
Cr ^{iv} —In3—In3 ⁱ	57.447 (8)	Tl2 ⁱ —Se4—Se3 ^{xx}	162.88 (2)
Cr ^{iv} —In3—In3 ⁱⁱ	122.553 (14)	Tl2 ⁱ —Se4—Se3 ^v	73.913 (13)
Cr ^{iv} —In3—Se1	146.097 (7)	Tl2 ⁱ —Se4—Se3 ^{vi}	110.197 (19)
Cr ^{iv} —In3—Se1 ^{xii}	81.246 (13)	Tl2 ⁱ —Se4—Se4 ⁱ	52.785 (10)
Cr ^{iv} —In3—Se1 ^{xiii}	117.067 (18)	Tl2 ⁱ —Se4—Se4 ⁱⁱ	127.215 (17)
Cr ^{iv} —In3—Se3 ^{xv}	47.199 (12)	Tl2—Se4—In1 ^{xviii}	118.427 (18)
Cr ^{iv} —In3—Se4 ^v	47.930 (17)	Tl2—Se4—Cr ^{xviii}	118.427 (18)
Cr ^{iv} —In3—Se4 ^{vi}	98.44 (2)	Tl2—Se4—In3 ^v	153.93 (3)
Cr ^{vii} —In3—In3 ⁱ	122.553 (14)	Tl2—Se4—In3 ^{vi}	88.858 (13)
Cr ^{vii} —In3—In3 ⁱⁱ	57.447 (8)	Tl2—Se4—Se2	65.299 (14)
Cr ^{vii} —In3—Se1	146.097 (7)	Tl2—Se4—Se3 ^{xix}	162.88 (2)
Cr ^{vii} —In3—Se1 ^{xii}	117.067 (18)	Tl2—Se4—Se3 ^{xx}	109.398 (10)
Cr ^{vii} —In3—Se1 ^{xiii}	81.246 (13)	Tl2—Se4—Se3 ^v	110.197 (19)
Cr ^{vii} —In3—Se3 ^{xv}	47.199 (12)	Tl2—Se4—Se3 ^{vi}	73.913 (13)

Cr ^{vii} —In ₃ —Se ^{4v}	98.44 (2)	Tl ₂ —Se ₄ —Se ⁴ⁱ	127.215 (17)
Cr ^{vii} —In ₃ —Se ^{4vi}	47.930 (17)	Tl ₂ —Se ₄ —Se ⁴ⁱⁱ	52.785 (10)
In ₃ ⁱ —In ₃ —In ₃ ⁱⁱ	180.0 (5)	In ^{xviii} —Se ₄ —Cr ^{xviii}	0.0 (5)
In ₃ ⁱ —In ₃ —Se ^{1xii}	55.649 (9)	In ^{xviii} —Se ₄ —In ₃ ^v	87.01 (2)
In ₃ ⁱ —In ₃ —Se ^{1xiii}	124.351 (13)	In ^{xviii} —Se ₄ —In ₃ ^{vi}	87.01 (2)
In ₃ ⁱ —In ₃ —Se ^{4v}	40.619 (12)	In ^{xviii} —Se ₄ —Se ₂	174.94 (2)
In ₃ ⁱ —In ₃ —Se ^{4vi}	139.381 (18)	In ^{xviii} —Se ₄ —Se ₃ ^{xix}	44.701 (13)
In ₃ ⁱⁱ —In ₃ —Se ^{1xii}	124.351 (13)	In ^{xviii} —Se ₄ —Se ₃ ^{xx}	44.701 (13)
In ₃ ⁱⁱ —In ₃ —Se ^{1xiii}	55.649 (9)	In ^{xviii} —Se ₄ —Se ₃ ^v	44.590 (12)
In ₃ ⁱⁱ —In ₃ —Se ^{4v}	139.381 (18)	In ^{xviii} —Se ₄ —Se ₃ ^{vi}	44.590 (12)
In ₃ ⁱⁱ —In ₃ —Se ^{4vi}	40.619 (12)	In ^{xviii} —Se ₄ —Se ⁴ⁱ	90.000 (14)
Se ₁ —In ₃ —Se ^{1xii}	71.494 (18)	In ^{xviii} —Se ₄ —Se ⁴ⁱⁱ	90.000 (14)
Se ₁ —In ₃ —Se ^{1xiii}	71.494 (18)	Cr ^{xviii} —Se ₄ —In ₃ ^v	87.01 (2)
Se ₁ —In ₃ —Se ₃ ^{xv}	133.67 (3)	Cr ^{xviii} —Se ₄ —In ₃ ^{vi}	87.01 (2)
Se ₁ —In ₃ —Se ^{4v}	113.92 (2)	Cr ^{xviii} —Se ₄ —Se ₂	174.94 (2)
Se ₁ —In ₃ —Se ^{4vi}	113.92 (2)	Cr ^{xviii} —Se ₄ —Se ₃ ^{xix}	44.701 (13)
Se ^{1xii} —In ₃ —Se ^{1xiii}	68.701 (13)	Cr ^{xviii} —Se ₄ —Se ₃ ^{xx}	44.701 (13)
Se ^{1xii} —In ₃ —Se ₃ ^{xv}	70.606 (18)	Cr ^{xviii} —Se ₄ —Se ₃ ^v	44.590 (12)
Se ^{1xii} —In ₃ —Se ^{4v}	95.083 (14)	Cr ^{xviii} —Se ₄ —Se ₃ ^{vi}	44.590 (12)
Se ^{1xii} —In ₃ —Se ^{4vi}	160.95 (2)	Cr ^{xviii} —Se ₄ —Se ⁴ⁱ	90.000 (14)
Se ^{1xiii} —In ₃ —Se ₃ ^{xv}	70.606 (18)	Cr ^{xviii} —Se ₄ —Se ⁴ⁱⁱ	90.000 (14)
Se ^{1xiii} —In ₃ —Se ^{4v}	160.95 (2)	In ₃ ^v —Se ₄ —In ₃ ^{vi}	98.76 (2)
Se ^{1xiii} —In ₃ —Se ^{4vi}	95.083 (14)	In ₃ ^v —Se ₄ —Se ₂	89.70 (2)
Se ₃ ^{xv} —In ₃ —Se ^{4v}	95.08 (2)	In ₃ ^v —Se ₄ —Se ₃ ^{xix}	42.356 (17)
Se ₃ ^{xv} —In ₃ —Se ^{4vi}	95.08 (2)	In ₃ ^v —Se ₄ —Se ₃ ^{xx}	92.50 (2)
Se ^{4v} —In ₃ —Se ^{4vi}	98.76 (2)	In ₃ ^v —Se ₄ —Se ₃ ^v	83.236 (17)
In ₂ ^v —Se ₁ —In ₂ ^{vi}	92.86 (2)	In ₃ ^v —Se ₄ —Se ₃ ^{vi}	131.55 (3)
In ₂ ^v —Se ₁ —In ₃	112.287 (19)	In ₃ ^v —Se ₄ —Se ⁴ⁱ	40.619 (12)
In ₂ ^v —Se ₁ —In ₃ ^{xii}	84.802 (14)	In ₃ ^v —Se ₄ —Se ⁴ⁱⁱ	139.38 (2)
In ₂ ^v —Se ₁ —In ₃ ^{xiii}	136.64 (2)	In ₃ ^{vi} —Se ₄ —Se ₂	89.70 (2)
In ₂ ^v —Se ₁ —Se ¹ⁱ	43.568 (12)	In ₃ ^{vi} —Se ₄ —Se ₃ ^{xix}	92.50 (2)
In ₂ ^v —Se ₁ —Se ¹ⁱⁱ	136.43 (2)	In ₃ ^{vi} —Se ₄ —Se ₃ ^{xx}	42.356 (17)
In ₂ ^v —Se ₁ —Se ^{1xii}	100.184 (12)	In ₃ ^{vi} —Se ₄ —Se ₃ ^v	131.55 (3)
In ₂ ^v —Se ₁ —Se ^{1xiii}	166.119 (16)	In ₃ ^{vi} —Se ₄ —Se ₃ ^{vi}	83.236 (17)
In ₂ ^v —Se ₁ —Se ₂	47.575 (13)	In ₃ ^{vi} —Se ₄ —Se ⁴ⁱ	139.38 (2)
In ₂ ^v —Se ₁ —Se ₃ ^x	54.788 (16)	In ₃ ^{vi} —Se ₄ —Se ⁴ⁱⁱ	40.619 (12)
In ₂ ^v —Se ₁ —Se ₃ ^{xi}	102.65 (2)	Se ₂ —Se ₄ —Se ₃ ^{xix}	131.745 (18)
In ₂ ^{vi} —Se ₁ —In ₃	112.287 (19)	Se ₂ —Se ₄ —Se ₃ ^{xx}	131.745 (18)
In ₂ ^{vi} —Se ₁ —In ₃ ^{xii}	136.64 (2)	Se ₂ —Se ₄ —Se ₃ ^v	138.720 (15)
In ₂ ^{vi} —Se ₁ —In ₃ ^{xiii}	84.802 (14)	Se ₂ —Se ₄ —Se ₃ ^{vi}	138.720 (15)
In ₂ ^{vi} —Se ₁ —Se ¹ⁱ	136.43 (2)	Se ₂ —Se ₄ —Se ⁴ⁱ	90.000 (14)
In ₂ ^{vi} —Se ₁ —Se ¹ⁱⁱ	43.568 (12)	Se ₂ —Se ₄ —Se ⁴ⁱⁱ	90.000 (14)
In ₂ ^{vi} —Se ₁ —Se ^{1xii}	166.119 (16)	Se ₃ ^{xix} —Se ₄ —Se ₃ ^{xx}	62.063 (14)
In ₂ ^{vi} —Se ₁ —Se ^{1xiii}	100.184 (12)	Se ₃ ^{xix} —Se ₄ —Se ₃ ^v	57.123 (15)
In ₂ ^{vi} —Se ₁ —Se ₂	47.575 (13)	Se ₃ ^{xix} —Se ₄ —Se ₃ ^{vi}	89.291 (19)
In ₂ ^{vi} —Se ₁ —Se ₃ ^x	102.65 (2)	Se ₃ ^{xix} —Se ₄ —Se ⁴ⁱ	58.969 (12)
In ₂ ^{vi} —Se ₁ —Se ₃ ^{xi}	54.788 (16)	Se ₃ ^{xix} —Se ₄ —Se ⁴ⁱⁱ	121.031 (18)
In ₃ —Se ₁ —In ₃ ^{xii}	108.51 (2)	Se ₃ ^{xx} —Se ₄ —Se ₃ ^v	89.291 (19)

In3—Se1—In3 ^{xiii}	108.51 (2)	Se3 ^{xx} —Se4—Se3 ^{vi}	57.123 (15)
In3—Se1—Se1 ^{xiii}	67.047 (18)	Se3 ^{xx} —Se4—Se4 ⁱ	121.031 (18)
In3—Se1—Se2	135.19 (2)	Se3 ^{xx} —Se4—Se4 ⁱⁱ	58.969 (12)
In3—Se1—Se3 ^x	143.728 (13)	Se3 ^v —Se4—Se3 ^{vi}	61.929 (14)
In3—Se1—Se3 ^{xi}	143.728 (13)	Se3 ^v —Se4—Se4 ⁱ	59.036 (13)
In3 ^{xii} —Se1—In3 ^{xiii}	68.701 (13)	Se3 ^v —Se4—Se4 ⁱⁱ	120.964 (19)
In3 ^{xii} —Se1—Se1 ⁱ	55.649 (10)	Se3 ^{vi} —Se4—Se4 ⁱ	120.964 (19)
In3 ^{xii} —Se1—Se1 ⁱⁱ	124.351 (15)	Se3 ^{vi} —Se4—Se4 ⁱⁱ	59.036 (13)
In3 ^{xii} —Se1—Se1 ^{xiii}	41.459 (14)	Se4 ⁱ —Se4—Se4 ⁱⁱ	180.0 (5)

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$; (iii) $-x+1, y, -z+1$; (iv) $x+1/2, y-1/2, z$; (v) $-x+1/2, y-1/2, -z+1$; (vi) $-x+1/2, y+1/2, -z+1$; (vii) $x+1/2, y+1/2, z$; (viii) $-x, y, -z+1$; (ix) $-x, y+1, -z+1$; (x) $x-1/2, y-1/2, z$; (xi) $x-1/2, y+1/2, z$; (xii) $-x+1/2, y-1/2, -z$; (xiii) $-x+1/2, y+1/2, -z$; (xiv) $x, y, z-1$; (xv) $-x+1, y, -z$; (xvi) $x+1/2, y-1/2, z-1$; (xvii) $x+1/2, y+1/2, z-1$; (xviii) $x, y, z+1$; (xix) $x-1/2, y-1/2, z+1$; (xx) $x-1/2, y+1/2, z+1$.