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# Substitution of indium for chromium in $TlIn_{5-x}Cr_xSe_8$: crystal structure of $TlIn_{4.811(5)}Cr_{0.189(5)}Se_8$

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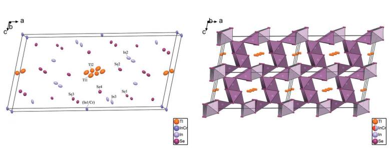
The new thallium penta(indium/chromium) octaselenide, $TlIn_{4.811(5)}Cr_{0.189(5)}Se_8$, has been synthesized by solid-state reaction. It crystallizes isotypically with $TlIn_5Se_8$ in the space group *C*2/*m*. Although the two Tl positions are disordered and only partially occupied, no Tl deficiency 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 2*a*). In the crystal structure, edge-sharing $InSe_6$ octahedra, and $(In,Cr)Se_6$ 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 $Ba_{0.5}Cr_5Se_8$ have thermal conductivities well below 1 W m$^{-1}$ 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 $TlV_{5-x}Cr_xSe_8$ ($x$ = 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 $TlIn_{5-x}Cr_xSe_8$. Initially, the nominal composition $TlIn_4CrSe_8$ was chosen so that chromium fully substitutes indium at the octahedral site (Wyckoff position 2*a*) of $TlIn_5Se_8$. Here we present the structure of one compound of the solid solution series

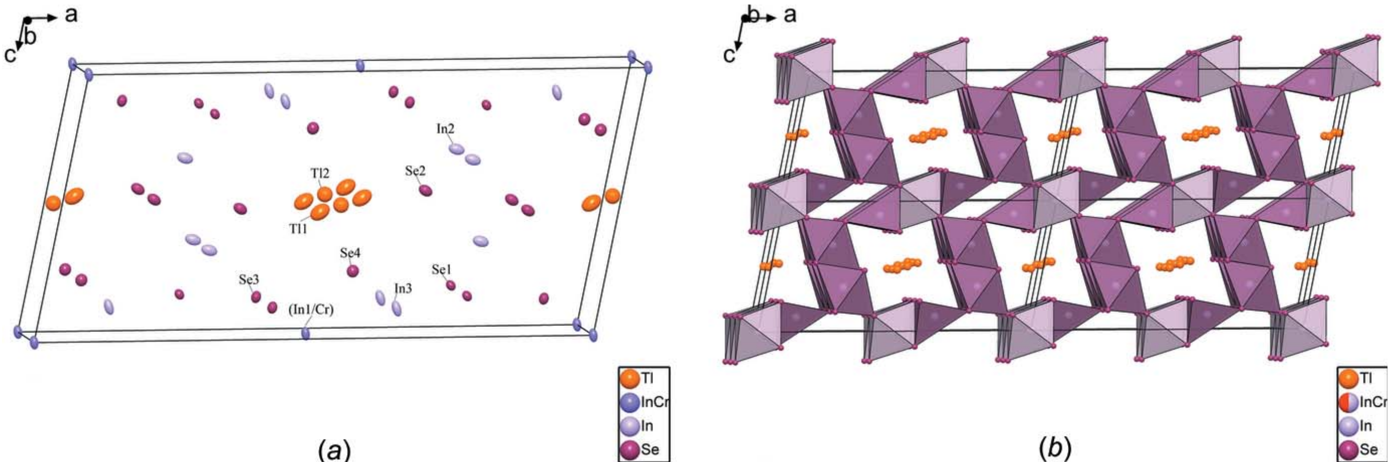



**Figure 1**
The crystal structure of $TlIn_{4.811(5)}Cr_{0.189(5)}Se_8$. (*a*) Representation by atoms displayed with displacement ellipsoids at the 50% probability level; (*b*) polyhedral representation.

$TlIn_{5-x}Cr_xSe_8$ ($x$ = 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 Tl, one mixed-occupied In/Cr, two In and four Se sites) are located on special positions. Except Tl2 and mixed-occupied (In1/Cr) on positions with site symmetry 2/*m* (Wyckoff positions 2*d* and 2*a*, respectively), all other atoms are located on a mirror plane (4*i*).

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 $(In1,Cr)Se_6$ 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 $(In1/Cr)Se_6$ 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 Tl 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 $TlIn_{5-x}Cr_xSe_8$ from $x = 0$ (Walther & Deiseroth, 1998) to $x = 5$ (Klepp & Boller, 1983), as explicited 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; Tl (granules, 99.99%), as well from Alfa Aesar, received in water, was first rinsed and dried before being stored in a glovebox. The elements Tl, In, Cr and Se in the molar ratio 1:4:1:8 were

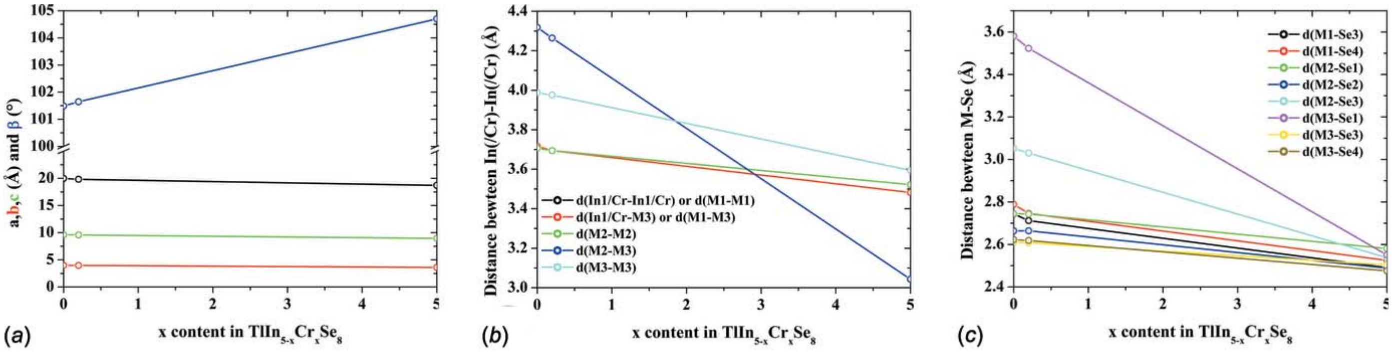



**Figure 2**
Evolution of (*a*) the unit-cell parameters, (*b*) $M$—$M$ distances and (*c*) $M$—Se distances depending on $x$ in the $TlIn_{5-x}Cr_xSe_8$ solid solution series.

**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, *C*2/*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*α |
| 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 |
| $(\sin \theta/\lambda)_{max}$ (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 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (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 $TlCr_5Se_8$ (Klepp & Boller, 1983) and $TlIn_5Se_8$ (Walther & Deiseroth, 1998). However, the Bragg positions of these reflections were clearly shifted, pointing to the presence of a $TlIn_{5-x}Cr_xSe_8$ 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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## References

Brandenburg, K. & Putz, H. (2014). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Klepp, K. & Boller, H. (1983). *J. Solid State Chem.* **48**, 388–395.
Lefèvre, R., Berthebaud, D., Bux, S., Hébert, S. & Gascoin, F. (2016). *Dalton Trans.* **45**, 12119–12126.
Lefèvre, R., Berthebaud, D., Perez, O., Pelloquin, D., Hébert, S. & Gascoin, F. (2015). *Chem. Mater.* **27**, 7110–7118.
Maier, S., Lefèvre, R., Lin, X., Nunna, R., Berthebaud, D., Hèbert, S., Mar, A. & Gascoin, F. (2015). *J. Mater. Chem. C.* **3**, 10509–10517.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Panalytical (2009). *X'Pert HighScore plus 3.0*. Panalytical B. V., Almelo, The Netherlands.
Petříček, V., Dušek, M. & Palatinus, L. (2014). *Z. Kristallogr.* **229**, 345–352.
Takahashi, H., Raghavendra, N., Gascoin, F., Pelloquin, D., Hébert, S. & Guilmeau, E. (2013). *Chem. Mater.* **25**, 1809–1815.
Walther, R. & Deiseroth, H. J. (1998). *Z. Krist. New Cryst. Struct.* **212**, 293.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

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### Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (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*

$TlIn_{4.811}Cr_{0.189}Se_8$
$M_r$ = 1398.3
Monoclinic, $C2/m$
Hall symbol: -C 2y
$a$ = 19.8257 (18) Å
$b$ = 3.9754 (4) Å
$c$ = 9.5881 (9) Å
$\beta$ = 101.645 (5)°
$V$ = 740.13 (12) Å$^3$
$Z$ = 2
$F(000)$ = 1187
$D_x$ = 6.274 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2692 reflections
$\theta$ = 2.7–32.8°
$\mu$ = 37.98 mm$^{-1}$
$T$ = 293 K
Irregular, black
0.13 × 0.11 × 0.10 mm

*Data collection*

Bruker APEXII CCD area detector diffractometer
Radiation source: X-ray tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: numerical (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.405, $T_{max}$ = 0.747
5647 measured reflections
1537 independent reflections
1181 reflections with $I > 3\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 33.2°, $\theta_{min}$ = 2.1°
$h = -30 \rightarrow 26$
$k = -5 \rightarrow 6$
$l = -12 \rightarrow 14$

*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 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.69 e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, º)*

| | | | |
|---|---|---|---|
| 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$^{xii}$—Se1—Se2 | 142.961 (13) |

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| 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) |

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| 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) |

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| $Se4^{ii}$—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) |

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

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| 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$^{viii}$ | 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$^{viii}$ | 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$^{viii}$ | 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) |

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| $In3^{xiii}$—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—$Se4^{viii}$ | 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—$Se4^{viii}$ | 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—$Se4^{viii}$ | 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—$Se4^{viii}$ | 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—$Se4^{viii}$ | 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) |

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| 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) |

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|---|---|---|---|
| $Cr^{vii}$—In3—$Se4^{v}$ | 98.44 (2) | Tl2—Se4—$Se4^{i}$ | 127.215 (17) |
| $Cr^{vii}$—In3—$Se4^{vi}$ | 47.930 (17) | Tl2—Se4—$Se4^{ii}$ | 52.785 (10) |
| $In3^{i}$—In3—$In3^{ii}$ | 180.0 (5) | $In1^{xviii}$—Se4—$Cr^{xviii}$ | 0.0 (5) |
| $In3^{i}$—In3—$Se1^{xii}$ | 55.649 (9) | $In1^{xviii}$—Se4—$In3^{v}$ | 87.01 (2) |
| $In3^{i}$—In3—$Se1^{xiii}$ | 124.351 (13) | $In1^{xviii}$—Se4—$In3^{vi}$ | 87.01 (2) |
| $In3^{i}$—In3—$Se4^{v}$ | 40.619 (12) | $In1^{xviii}$—Se4—Se2 | 174.94 (2) |
| $In3^{i}$—In3—$Se4^{vi}$ | 139.381 (18) | $In1^{xviii}$—Se4—$Se3^{xix}$ | 44.701 (13) |
| $In3^{ii}$—In3—$Se1^{xii}$ | 124.351 (13) | $In1^{xviii}$—Se4—$Se3^{xx}$ | 44.701 (13) |
| $In3^{ii}$—In3—$Se1^{xiii}$ | 55.649 (9) | $In1^{xviii}$—Se4—$Se3^{v}$ | 44.590 (12) |
| $In3^{ii}$—In3—$Se4^{v}$ | 139.381 (18) | $In1^{xviii}$—Se4—$Se3^{vi}$ | 44.590 (12) |
| $In3^{ii}$—In3—$Se4^{vi}$ | 40.619 (12) | $In1^{xviii}$—Se4—$Se4^{i}$ | 90.000 (14) |
| Se1—In3—$Se1^{xii}$ | 71.494 (18) | $In1^{xviii}$—Se4—$Se4^{ii}$ | 90.000 (14) |
| Se1—In3—$Se1^{xiii}$ | 71.494 (18) | $Cr^{xviii}$—Se4—$In3^{v}$ | 87.01 (2) |
| Se1—In3—$Se3^{xv}$ | 133.67 (3) | $Cr^{xviii}$—Se4—$In3^{vi}$ | 87.01 (2) |
| Se1—In3—$Se4^{v}$ | 113.92 (2) | $Cr^{xviii}$—Se4—Se2 | 174.94 (2) |
| Se1—In3—$Se4^{vi}$ | 113.92 (2) | $Cr^{xviii}$—Se4—$Se3^{xix}$ | 44.701 (13) |
| $Se1^{xii}$—In3—$Se1^{xiii}$ | 68.701 (13) | $Cr^{xviii}$—Se4—$Se3^{xx}$ | 44.701 (13) |
| $Se1^{xii}$—In3—$Se3^{xv}$ | 70.606 (18) | $Cr^{xviii}$—Se4—$Se3^{v}$ | 44.590 (12) |
| $Se1^{xii}$—In3—$Se4^{v}$ | 95.083 (14) | $Cr^{xviii}$—Se4—$Se3^{vi}$ | 44.590 (12) |
| $Se1^{xii}$—In3—$Se4^{vi}$ | 160.95 (2) | $Cr^{xviii}$—Se4—$Se4^{i}$ | 90.000 (14) |
| $Se1^{xiii}$—In3—$Se3^{xv}$ | 70.606 (18) | $Cr^{xviii}$—Se4—$Se4^{ii}$ | 90.000 (14) |
| $Se1^{xiii}$—In3—$Se4^{v}$ | 160.95 (2) | $In3^{v}$—Se4—$In3^{vi}$ | 98.76 (2) |
| $Se1^{xiii}$—In3—$Se4^{vi}$ | 95.083 (14) | $In3^{v}$—Se4—Se2 | 89.70 (2) |
| $Se3^{xv}$—In3—$Se4^{v}$ | 95.08 (2) | $In3^{v}$—Se4—$Se3^{xix}$ | 42.356 (17) |
| $Se3^{xv}$—In3—$Se4^{vi}$ | 95.08 (2) | $In3^{v}$—Se4—$Se3^{xx}$ | 92.50 (2) |
| $Se4^{v}$—In3—$Se4^{vi}$ | 98.76 (2) | $In3^{v}$—Se4—$Se3^{v}$ | 83.236 (17) |
| $In2^{v}$—Se1—$In2^{vi}$ | 92.86 (2) | $In3^{v}$—Se4—$Se3^{vi}$ | 131.55 (3) |
| $In2^{v}$—Se1—In3 | 112.287 (19) | $In3^{v}$—Se4—$Se4^{i}$ | 40.619 (12) |
| $In2^{v}$—Se1—$In3^{xii}$ | 84.802 (14) | $In3^{v}$—Se4—$Se4^{ii}$ | 139.38 (2) |
| $In2^{v}$—Se1—$In3^{xiii}$ | 136.64 (2) | $In3^{vi}$—Se4—Se2 | 89.70 (2) |
| $In2^{v}$—Se1—$Se1^{i}$ | 43.568 (12) | $In3^{vi}$—Se4—$Se3^{xix}$ | 92.50 (2) |
| $In2^{v}$—Se1—$Se1^{ii}$ | 136.43 (2) | $In3^{vi}$—Se4—$Se3^{xx}$ | 42.356 (17) |
| $In2^{v}$—Se1—$Se1^{xii}$ | 100.184 (12) | $In3^{vi}$—Se4—$Se3^{v}$ | 131.55 (3) |
| $In2^{v}$—Se1—$Se1^{xiii}$ | 166.119 (16) | $In3^{vi}$—Se4—$Se3^{vi}$ | 83.236 (17) |
| $In2^{v}$—Se1—Se2 | 47.575 (13) | $In3^{vi}$—Se4—$Se4^{i}$ | 139.38 (2) |
| $In2^{v}$—Se1—$Se3^{x}$ | 54.788 (16) | $In3^{vi}$—Se4—$Se4^{ii}$ | 40.619 (12) |
| $In2^{v}$—Se1—$Se3^{xi}$ | 102.65 (2) | Se2—Se4—$Se3^{xix}$ | 131.745 (18) |
| $In2^{vi}$—Se1—In3 | 112.287 (19) | Se2—Se4—$Se3^{xx}$ | 131.745 (18) |
| $In2^{vi}$—Se1—$In3^{xii}$ | 136.64 (2) | Se2—Se4—$Se3^{v}$ | 138.720 (15) |
| $In2^{vi}$—Se1—$In3^{xiii}$ | 84.802 (14) | Se2—Se4—$Se3^{vi}$ | 138.720 (15) |
| $In2^{vi}$—Se1—$Se1^{i}$ | 136.43 (2) | Se2—Se4—$Se4^{i}$ | 90.000 (14) |
| $In2^{vi}$—Se1—$Se1^{ii}$ | 43.568 (12) | Se2—Se4—$Se4^{ii}$ | 90.000 (14) |
| $In2^{vi}$—Se1—$Se1^{xii}$ | 166.119 (16) | $Se3^{xix}$—Se4—$Se3^{xx}$ | 62.063 (14) |
| $In2^{vi}$—Se1—$Se1^{xiii}$ | 100.184 (12) | $Se3^{xix}$—Se4—$Se3^{v}$ | 57.123 (15) |
| $In2^{vi}$—Se1—Se2 | 47.575 (13) | $Se3^{xix}$—Se4—$Se3^{vi}$ | 89.291 (19) |
| $In2^{vi}$—Se1—$Se3^{x}$ | 102.65 (2) | $Se3^{xix}$—Se4—$Se4^{i}$ | 58.969 (12) |
| $In2^{vi}$—Se1—$Se3^{xi}$ | 54.788 (16) | $Se3^{xix}$—Se4—$Se4^{ii}$ | 121.031 (18) |
| In3—Se1—$In3^{xii}$ | 108.51 (2) | $Se3^{xx}$—Se4—$Se3^{v}$ | 89.291 (19) |

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| 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$^{xii}$ | 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.