Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Thallium(I) copper(I) thorium(IV) triselenide, $TlCuThSe_3$

Lukasz A. Koscielski and James A. Ibers*

Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3113, USA
Correspondence e-mail: ibers@chem.northwestern.edu

Received 1 June 2012; accepted 12 June 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(Se–Cu) = 0.001 Å; R factor = 0.021; wR factor = 0.046; data-to-parameter ratio = 19.8.

Thallium(I) copper(I) thorium(IV) triselenide, $TlCuThSe_3$, crystallizes with four formula units in the space group *Cmcm* in the $KCuZrS_3$ structure type. There is one crystallographically independent Th, Tl, and Cu atom at a site of symmetry $2/m$.., $m2m$, and $m2m$, respectively. There are two crystallographically independent Se atoms at sites of symmetry m.. and $m2m$. The structure consists of sheets of edge-sharing $ThSe_6$ octahedra and $CuSe_4$ tetrahedra stacked parallel to the (010) face, separated by layers filled with chains of Tl running parallel to [100]. Each Tl is coordinated by a trigonal prism of Se atoms.

Related literature

For compounds of type $AMM'Q_3$, see: Pell & Ibers (1996); Klepp & Gurtner (1996) for A = Tl; Pell *et al.* (1997); Yao *et al.* (2008); Wells *et al.* (2009) for M = Ag; Bugaris & Ibers (2009) for M = Au; Mansuetto *et al.* (1993); Pell & Ibers (1996) for M' = Ti; Mansuetto *et al.* (1992, 1993); Huang *et al.* (2001); Pell *et al.* (1997) for M' = Zr; Klepp & Sturmayr (1997, 1998); Pell *et al.* (1997) for M' = Hf; Seldy *et al.* (2005); Narducci & Ibers (2000) for M' = Th; Yao *et al.* (2008); Sutorik *et al.* (1996); Bugaris & Ibers (2009); Huang *et al.* (2001); Cody & Ibers (1995) for M' = U; Wells *et al.* (2009) for M' = Np. For computational details, see: Gelato & Parthé (1987). For additional synthetic details, see: Witt *et al.* (1956).

Experimental

Crystal data

$TlCuThSe_3$
M_r = 736.83
Orthorhombic, *Cmcm*
a = 4.1678 (2) Å
b = 14.2227 (7) Å
c = 10.8476 (5) Å
V = 643.02 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 68.19 mm^{-1}
T = 100 K
0.10 × 0.07 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: numerical (*SADABS*; Sheldrick, 2008*b*)
T_{min} = 0.101, T_{max} = 0.489
7476 measured reflections
474 independent reflections
451 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.046
S = 1.59
474 reflections
24 parameters
$\Delta\rho_{max}$ = 2.01 e Å^{-3}
$\Delta\rho_{min}$ = −1.34 e Å^{-3}

Table 1
Selected bond lengths (Å).

Th1—Se2^{i}	2.8844 (4)	Tl1—Se1^{viii}	3.3564 (6)
Th1—Se2	2.8844 (4)	Tl1—Se1^{vi}	3.3564 (6)
Th1—Se1^{ii}	2.9057 (5)	Tl1—Se1^{ix}	3.3564 (6)
Th1—Se1^{iii}	2.9057 (5)	Tl1—Se1^{vii}	3.3564 (6)
Th1—Se1^{iv}	2.9057 (5)	Cu1—Se1	2.4617 (11)
Th1—Se1^{v}	2.9057 (5)	Cu1—Se1^{x}	2.4617 (11)
Tl1—Se2^{vi}	3.2831 (9)	Cu1—Se2^{vii}	2.5517 (11)
Tl1—Se2^{vii}	3.2831 (9)	Cu1—Se2^{vi}	2.5517 (11)

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (iii) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $-x-\frac{1}{2}, -y+\frac{1}{2}, -z$; (v) $x+\frac{1}{2}, y-\frac{1}{2}, z$; (vi) $x-\frac{1}{2}, y+\frac{1}{2}, z$; (vii) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (viii) $x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ix) $x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (x) $x, y, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*a*); molecular graphics: *CrystalMaker* (Palmer, 2009); software used to prepare material for publication: *SHELXL97*.

The research was supported at Northwestern University by the U. S. Department of Energy, Basic Energy Sciences, Chemical Sciences, Biosciences, and Geosciences Division and Division of Materials Sciences and Engineering Grant ER-15522. The research was also supported by funding received from the DOE Office of Nuclear Energy's Nuclear Energy University Programs. A special thanks to Professor Thomas E. Albrecht-Schmitt at the University of Notre-Dame for his donation of thorium metal.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2644).

References

Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bugaris, D. E. & Ibers, J. A. (2009). *J. Solid State Chem.* **182**, 2587–2590.
Cody, J. A. & Ibers, J. A. (1995). *Inorg. Chem.* **34**, 3165–3172.
Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
Huang, F.-Q., Mitchell, K. & Ibers, J. A. (2001). *Inorg. Chem.* **40**, 5123–5126.
Klepp, K. O. & Gurtner, D. (1996). *J. Alloys Compd*, **243**, 6–11.
Klepp, K. O. & Sturmayr, D. (1997). *Z. Kristallogr. New Cryst. Struct.* **212**, 75.
Klepp, K. O. & Sturmayr, D. (1998). *Z. Kristallogr. New Cryst. Struct.* **213**, 693.
Mansuetto, M. F., Keane, P. M. & Ibers, J. A. (1992). *J. Solid State Chem.* **101**, 257–264.
Mansuetto, M. F., Keane, P. M. & Ibers, J. A. (1993). *J. Solid State Chem.* **105**, 580–587.
Narducci, A. A. & Ibers, J. A. (2000). *Inorg. Chem.* **39**, 688–691.
Palmer, D. (2009). *CrystalMaker*. CrystalMaker Software Ltd, Oxfordshire, England.

Pell, M. A. & Ibers, J. A. (1996). *J. Alloys Compd*, **240**, 37–41.

Pell, M. A., Kleyn, A. G. & Ibers, J. A. (1997). *Z. Kristallogr. New Cryst. Struct.* **212**, 92–?.

Seldy, H. D., Chan, B. C., Hess, R. F., Abney, K. D. & Dorhout, P. K. (2005). *Inorg. Chem.* **44**, 6463–6469.

Sheldrick, G. M. (2008*a*). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2008*b*). *SADABS*. University of Göttingen, Germany.

Sutorik, A. C., Albritton-Thomas, J., Hogan, T., Kannewurf, C. R. & Kanatzidis, M. G. (1996). *Chem. Mater.* **8**, 751–761.

Wells, D. M., Jin, G. B., Skanthakumar, S., Haire, R. G., Soderholm, L. & Ibers, J. A. (2009). *Inorg. Chem.* **48**, 11513–11517.

Witt, R. H., Nylin, J. & McCullough, H. M. (1956). *A Study of the Hydride Process for Producing Thorium Powder.* United States Atomic Energy Commission, Atomic Energy Division, Sylvania Electric Products, Inc., Bayside, New York.

Yao, J., Wells, D. M., Chan, G.-H., Zeng, H., Ellis, D. E., van Duyne, R. P. & Ibers, J. A. (2008). *Inorg. Chem.* **47**, 6873–6879.

supplementary materials

Acta Cryst. (2012). E**68**, i52–i53   [doi:10.1107/S1600536812026669]

Thallium(I) copper(I) thorium(IV) triselenide, $TlCuThSe_3$

Lukasz A. Koscielski and James A. Ibers

Comment

Thallium(I) copper(I) thorium(IV) triselenide, $TlCuThSe_3$, crystallizes in the $KCuZrS_3$ structure type. The structure (Figs. 1, 2) is layered and consists of sheets of edge-sharing $ThSe_6$ octahedra and $CuSe_4$ tetrahedra stacked parallel to the (010) face separated by layers filled with chains of Tl running parallel to [100]. Each Tl is coordinated by a trigonal prism of Se atoms. Because there are no Se—Se bonds in the structure, oxidation states can be assigned as Tl^+, Cu^+, Th^{4+}, and Se^{2-}.

The compound $TlCuThSe_3$ is of the type $AMM'Q_3$, where A is an alkali metal or thallium, M is a coinage metal, M' is a tetravalent group IV metal or an actinide, and Q is a chalcogen. Including the title compound, 39 such compounds are known (Pell & Ibers, 1996; Klepp & Gurtner, 1996; Pell *et al.*, 1997; Yao *et al.*, 2008; Wells *et al.*, 2009; Bugaris & Ibers, 2009; Sutorik *et al.*, 1996; Huang *et al.*, 2001; Cody & Ibers, 1995; Mansuetto *et al.*, 1993, 1992; Klepp & Sturmayr, 1997, 1998; Seldy *et al.*, 2005; Narducci & Ibers, 2000). In all cases, crystallographic data have been collected on single crystals. Most often, the A site contains an alkali metal and only 6 Tl analogues are known (Pell & Ibers, 1996; Klepp & Gurtner, 1996). The M site contains Cu in 28 analogues, Ag in 7 analogues (Pell *et al.*, 1997; Yao *et al.*, 2008; Wells *et al.*, 2009), and Au in 4 analogues (Bugaris & Ibers, 2009). The tetravalent metal is most often U with 14 analogues (Yao *et al.*, 2008; Sutorik *et al.*, 1996; Bugaris & Ibers, 2009; Huang *et al.*, 2001; Cody & Ibers, 1995), followed by Zr with 9 analogues (Mansuetto *et al.*, 1992, 1993; Huang *et al.*, 2001; Pell *et al.*, 1997), Hf with 5 analogues (Klepp & Sturmayr, 1997, 1998; Pell *et al.*, 1997), Np with 5 analogues (Wells *et al.*, 2009), Th with 4 analogues (Seldy *et al.*, 2005; Narducci & Ibers, 2000), and Ti with 2 analogues (Mansuetto *et al.*, 1993; Pell & Ibers, 1996). This is the first compound of the type $AMM'Q_3$ to contain both Tl and Th.

The compounds fall into three structure types. All the Na analogues, except for $NaCuZrS_3$, are of the $NaCuTiS_3$ type (space group *Pnma*) (Mansuetto *et al.*, 1993; Klepp & Sturmayr, 1997); the compounds $TlCuTiTe_3$ and $RbAgHfTe_3$ are of the $TlCuTiTe_3$ type (space group $P2_1/m$) (Pell & Ibers, 1996; Pell *et al.*, 1997); and the remaining compounds are of the $KCuZrS_3$ type (space group *Cmcm*).

Interatomic distances in $TlCuThSe_3$ are listed in Table 1 and are nearly identical to those in the analogues $ACuThSe_3$ (A = K, Cs) (Narducci & Ibers, 2000). The $TlCuThSe_3$ Th—Se distances of 2.8844 (4) and 2.9057 (5) Å match those in $KCuThSe_3$ (2.893 (1) and 2.900 (1) Å) and $CsCuThSe_3$ (2.878 (1) and 2.906 (1) Å). The Cu—Se distances of 2.4617 (11) and 2.5517 (11) Å also match those in $KCuThSe_3$ (2.459 (2) and 2.545 (2) Å) and $CsCuThSe_3$ (2.464 (2) and 2.556 (2) Å).

Experimental

Cu (Aldrich, 99.5%), Tl_2Se (Aldrich, 99.999%), and Se (Cerac, 99.999%) were used as received. Th chunks were powdered according to a literature procedure (Witt *et al.*, 1956). A fused-silica tube was loaded with Th (30 mg, 0.129 mmol), Cu (7.0 mg, 0.110 mmol), Tl_2Se (36.6 mg, 0.075 mmol), and Se (20.4 mg, 0.258 mmol), evacuated to near 10^{-4} Torr, flame sealed, and placed in a computer-controlled furnace. It was heated to 597 K in 3 h, kept at 597 K for 24 h, heated to 1073 K in 24 h, kept at 1073 K for 96 h, cooled to 597 K in 96 h, cooled to 547 in 24 h, and then rapidly cooled to 298 K in 3 h. The reaction produced orange-red plates of TlCuThSe$_3$. The elemental composition of the crystals was determined to be Tl/Cu/Th/Se in an approximate ratio of 1/1/1/3 on an EDX-equipped Hitachi S-3400 SEM.

Refinement

The structure was standardized by means of the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak (2.0 (3) e Å^{-3}) is 0.98 Å from atom Tl1 and the deepest hole (-1.3 (3) e Å^{-3}) is 1.96 Å from atom Se1.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*a*); molecular graphics: *CrystalMaker* (Palmer, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008*a*).

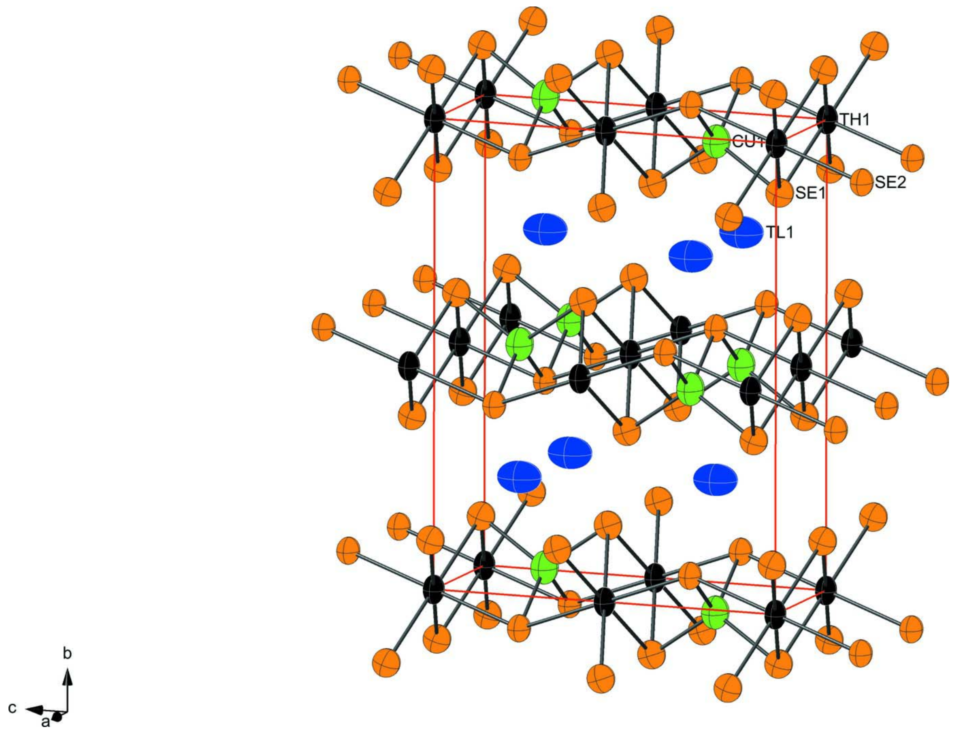

Figure 1

Structure of TlCuThSe$_3$ viewed approximately down the *a*-axis. The 95% probability displacement ellipsoids are depicted with the unit cell outlined in red. Color key: black – Th, green – Cu, blue – Tl, orange – Se.

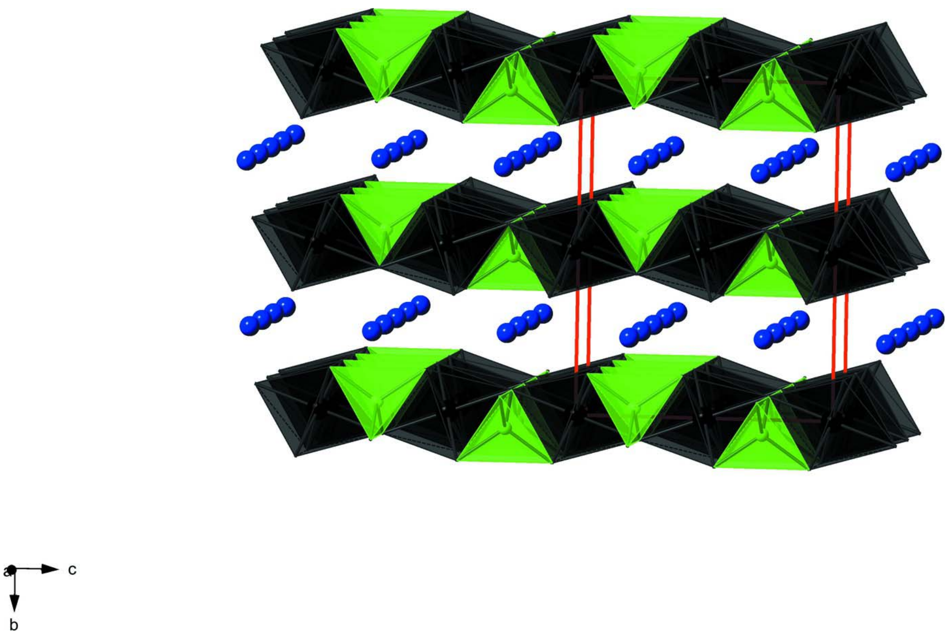

Figure 2

Polyhedral view of TlCuThSe$_3$ showing sheets of edge-sharing ThSe$_6$ octahedra (black) and CuSe$_4$ tetrahedra (green) separated by voids filled with Tl (blue). The unit cell is outlined in red.

Thallium(I) copper(I) thorium(IV) triselenide

Crystal data

TlCuThSe$_3$
M_r = 736.83
Orthorhombic, *Cmcm*
Hall symbol: -C 2c 2
a = 4.1678 (2) Å
b = 14.2227 (7) Å
c = 10.8476 (5) Å
V = 643.02 (5) Å^3
Z = 4

F(000) = 1208
D_x = 7.611 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1794 reflections
θ = 2.9–28.2°
μ = 68.19 mm^{-1}
T = 100 K
Rectangular plate, orange
0.10 × 0.07 × 0.02 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: numerical (*SADABS*; Sheldrick, 2008*b*)
$T_{\min}$ = 0.101, $T_{\max}$ = 0.489

7476 measured reflections
474 independent reflections
451 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
$\theta_{\max}$ = 28.5°, $\theta_{\min}$ = 2.9°
$h = -5 \rightarrow 5$
$k = -18 \rightarrow 18$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.046
S = 1.59

474 reflections
24 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[1.00000 + 0.00000\exp(0.00(\sin\theta/\lambda)^2)]/ [\sigma^2(F_o^2) + 0.0000 + 0.0000*P + (0.0193P)^2 + 0.0000\sin\theta/\lambda]$
where $P = 1.00000F_o^2 + 0.00000F_c^2$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.01$ e Å^{-3}
$\Delta\rho_{min} = -1.34$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008*a*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00066 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Th1	0.0000	0.0000	0.0000	0.00558 (15)
Tl1	0.0000	0.74746 (3)	0.2500	0.01247 (16)
Se1	0.0000	0.36628 (5)	0.06410 (7)	0.0067 (2)
Se2	0.0000	0.06909 (8)	0.2500	0.0059 (2)
Cu1	0.0000	0.46554 (10)	0.2500	0.0085 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Th1	0.0050 (2)	0.0078 (2)	0.0040 (2)	0.000	0.000	−0.00012 (14)
Tl1	0.0101 (3)	0.0092 (3)	0.0181 (3)	0.000	0.000	0.000
Se1	0.0062 (4)	0.0071 (4)	0.0067 (4)	0.000	0.000	−0.0002 (3)
Se2	0.0069 (5)	0.0064 (5)	0.0043 (5)	0.000	0.000	0.000
Cu1	0.0100 (7)	0.0096 (7)	0.0060 (6)	0.000	0.000	0.000

Geometric parameters (Å, º)

Th1—Se2^{i}	2.8844 (4)	Se1—Th1^{ix}	2.9057 (5)
Th1—Se2	2.8844 (4)	Se1—Th1^{viii}	2.9057 (5)
Th1—Se1^{ii}	2.9057 (5)	Se1—Tl1^{v}	3.3564 (6)
Th1—Se1^{iii}	2.9057 (5)	Se1—Tl1^{iii}	3.3564 (6)
Th1—Se1^{iv}	2.9057 (5)	Se1—Tl1^{xii}	3.7717 (8)
Th1—Se1^{v}	2.9057 (5)	Se1—Tl1^{xiv}	5.6211 (6)
Th1—Cu1^{iv}	3.4550 (2)	Se1—Tl1^{xv}	5.6211 (6)
Th1—Cu1^{v}	3.4550 (2)	Se2—Cu1^{iii}	2.5517 (11)
Th1—Cu1^{ii}	3.4550 (2)	Se2—Cu1^{v}	2.5517 (11)
Th1—Cu1^{iii}	3.4550 (2)	Se2—Th1^{xvi}	2.8844 (4)
Th1—Th1^{vi}	4.1678 (2)	Se2—Tl1^{v}	3.2831 (9)
Th1—Th1^{vii}	4.1678 (2)	Se2—Tl1^{iii}	3.2831 (9)
Tl1—Se2^{viii}	3.2831 (9)	Se2—Tl1^{xvii}	4.5744 (12)
Tl1—Se2^{ix}	3.2831 (9)	Cu1—Se1	2.4617 (11)

Tl1—Se1^{x}	3.3564 (6)	Cu1—Se1^{xviii}	2.4617 (11)
Tl1—Se1^{viii}	3.3564 (6)	Cu1—Se2^{ix}	2.5517 (11)
Tl1—Se1^{xi}	3.3564 (6)	Cu1—Se2^{viii}	2.5517 (11)
Tl1—Se1^{ix}	3.3564 (6)	Cu1—Th1^{xix}	3.4550 (2)
Tl1—Cu1^{ix}	3.7368 (13)	Cu1—Th1^{viii}	3.4550 (2)
Tl1—Cu1^{viii}	3.7368 (13)	Cu1—Th1^{xx}	3.4550 (2)
Tl1—Se1^{xii}	3.7717 (8)	Cu1—Th1^{ix}	3.4550 (2)
Tl1—Se1^{xiii}	3.7717 (8)	Cu1—Tl1^{iii}	3.7368 (13)
Tl1—Cu1	4.0095 (16)	Cu1—Tl1^{v}	3.7368 (13)
Tl1—Tl1^{vii}	4.1678 (2)		

Se2^{i}—Th1—Se2	180.0	Th1^{ix}—Se1—Tl1^{v}	91.607 (8)
Se2^{i}—Th1—Se1^{ii}	89.89 (2)	Th1^{viii}—Se1—Tl1^{v}	156.72 (3)
Se2—Th1—Se1^{ii}	90.11 (2)	Cu1—Se1—Tl1^{iii}	78.26 (3)
Se2^{i}—Th1—Se1^{iii}	90.11 (2)	Th1^{ix}—Se1—Tl1^{iii}	156.72 (3)
Se2—Th1—Se1^{iii}	89.89 (2)	Th1^{viii}—Se1—Tl1^{iii}	91.607 (8)
Se1^{ii}—Th1—Se1^{iii}	180.00 (4)	Tl1^{v}—Se1—Tl1^{iii}	76.761 (17)
Se2^{i}—Th1—Se1^{iv}	89.89 (2)	Cu1—Se1—Tl1^{xii}	170.40 (4)
Se2—Th1—Se1^{iv}	90.11 (2)	Th1^{ix}—Se1—Tl1^{xii}	93.702 (18)
Se1^{ii}—Th1—Se1^{iv}	91.64 (2)	Th1^{viii}—Se1—Tl1^{xii}	93.702 (18)
Se1^{iii}—Th1—Se1^{iv}	88.36 (2)	Tl1^{v}—Se1—Tl1^{xii}	109.076 (17)
Se2^{i}—Th1—Se1^{v}	90.11 (2)	Tl1^{iii}—Se1—Tl1^{xii}	109.076 (17)
Se2—Th1—Se1^{v}	89.89 (2)	Cu1—Se1—Tl1^{xiv}	131.422 (8)
Se1^{ii}—Th1—Se1^{v}	88.36 (2)	Th1^{ix}—Se1—Tl1^{xiv}	125.11 (2)
Se1^{iii}—Th1—Se1^{v}	91.64 (2)	Th1^{viii}—Se1—Tl1^{xiv}	60.762 (10)
Se1^{iv}—Th1—Se1^{v}	180.00 (4)	Tl1^{v}—Se1—Tl1^{xiv}	132.816 (19)
Se2^{viii}—Tl1—Se2^{ix}	78.80 (3)	Tl1^{iii}—Se1—Tl1^{xiv}	76.051 (8)
Se2^{viii}—Tl1—Se1^{x}	141.551 (14)	Tl1^{xii}—Se1—Tl1^{xiv}	47.856 (6)
Se2^{ix}—Tl1—Se1^{x}	89.713 (15)	Cu1—Se1—Tl1^{xv}	131.422 (9)
Se2^{viii}—Tl1—Se1^{viii}	89.713 (15)	Th1^{ix}—Se1—Tl1^{xv}	60.763 (10)
Se2^{ix}—Tl1—Se1^{viii}	141.551 (14)	Th1^{viii}—Se1—Tl1^{xv}	125.11 (2)
Se1^{x}—Tl1—Se1^{viii}	119.54 (3)	Tl1^{v}—Se1—Tl1^{xv}	76.051 (8)
Se2^{viii}—Tl1—Se1^{xi}	89.713 (15)	Tl1^{iii}—Se1—Tl1^{xv}	132.816 (19)
Se2^{ix}—Tl1—Se1^{xi}	141.551 (14)	Tl1^{xii}—Se1—Tl1^{xv}	47.856 (6)
Se1^{x}—Tl1—Se1^{xi}	76.760 (17)	Tl1^{xiv}—Se1—Tl1^{xv}	95.712 (12)
Se1^{viii}—Tl1—Se1^{xi}	73.86 (2)	Cu1^{iii}—Se2—Cu1^{v}	109.50 (7)
Se2^{viii}—Tl1—Se1^{ix}	141.551 (14)	Cu1^{iii}—Se2—Th1	78.662 (19)
Se2^{ix}—Tl1—Se1^{ix}	89.713 (15)	Cu1^{v}—Se2—Th1	78.662 (19)
Se1^{x}—Tl1—Se1^{ix}	73.86 (2)	Cu1^{iii}—Se2—Th1^{xvi}	78.662 (19)
Se1^{viii}—Tl1—Se1^{ix}	76.760 (17)	Cu1^{v}—Se2—Th1^{xvi}	78.662 (19)
Se1^{xi}—Tl1—Se1^{ix}	119.54 (3)	Th1—Se2—Th1^{xvi}	140.17 (4)
Se2^{viii}—Tl1—Se1^{xii}	70.645 (11)	Cu1^{iii}—Se2—Tl1^{v}	164.65 (4)
Se2^{ix}—Tl1—Se1^{xii}	70.645 (11)	Cu1^{v}—Se2—Tl1^{v}	85.85 (3)
Se1^{x}—Tl1—Se1^{xii}	139.351 (12)	Th1—Se2—Tl1^{v}	105.262 (13)
Se1^{viii}—Tl1—Se1^{xii}	70.924 (17)	Th1^{xvi}—Se2—Tl1^{v}	105.262 (13)
Se1^{xi}—Tl1—Se1^{xii}	139.351 (11)	Cu1^{iii}—Se2—Tl1^{iii}	85.85 (3)
Se1^{ix}—Tl1—Se1^{xii}	70.924 (17)	Cu1^{v}—Se2—Tl1^{iii}	164.65 (4)
Cu1^{ix}—Tl1—Se1^{xii}	110.855 (11)	Th1—Se2—Tl1^{iii}	105.262 (13)
Cu1^{viii}—Tl1—Se1^{xii}	110.855 (11)	Th1^{xvi}—Se2—Tl1^{iii}	105.262 (13)

Se2^{viii}—Tl1—Se1^{xiii}	70.645 (11)	Tl1^{v}—Se2—Tl1^{iii}	78.80 (3)
Se2^{ix}—Tl1—Se1^{xiii}	70.645 (11)	Cu1^{iii}—Se2—Tl1^{xvii}	54.75 (3)
Se1^{x}—Tl1—Se1^{xiii}	70.924 (17)	Cu1^{v}—Se2—Tl1^{xvii}	54.75 (3)
Se1^{viii}—Tl1—Se1^{xiii}	139.351 (11)	Th1—Se2—Tl1^{xvii}	70.08 (2)
Se1^{xi}—Tl1—Se1^{xiii}	70.924 (17)	Th1^{xvi}—Se2—Tl1^{xvii}	70.08 (2)
Se1^{ix}—Tl1—Se1^{xiii}	139.351 (11)	Tl1^{v}—Se2—Tl1^{xvii}	140.600 (14)
Cu1^{ix}—Tl1—Se1^{xiii}	110.855 (11)	Tl1^{iii}—Se2—Tl1^{xvii}	140.600 (14)
Cu1^{viii}—Tl1—Se1^{xiii}	110.855 (11)	Se1—Cu1—Se1^{xviii}	110.01 (7)
Se1^{xii}—Tl1—Se1^{xiii}	129.21 (3)	Se1—Cu1—Se2^{ix}	109.328 (14)
Cu1—Se1—Th1^{ix}	79.67 (3)	Se1^{xviii}—Cu1—Se2^{ix}	109.328 (14)
Cu1—Se1—Th1^{viii}	79.67 (3)	Se1—Cu1—Se2^{viii}	109.328 (14)
Th1^{ix}—Se1—Th1^{viii}	91.64 (2)	Se1^{xviii}—Cu1—Se2^{viii}	109.328 (14)
Cu1—Se1—Tl1^{v}	78.26 (3)	Se2^{ix}—Cu1—Se2^{viii}	109.51 (7)

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