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# $Tl_2Mo_9Se_{11}$

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Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(Mo–Se) = 0.001 Å; $R$ factor = 0.043; $wR$ factor = 0.092; data-to-parameter ratio = 59.4.

The structure of $Tl_2Mo_9Se_{11}$, dithallium nonamolybdenum undecaselenide, is isotypic with $Tl_2Mo_9S_{11}$ [Potel *et al.* (1980). *Acta Cryst.* B**36**, 1319–1322]. The structural set-up is characterized by a mixture of $Mo_6Se_8^iSe_6^a$ and $Mo_{12}Se_{14}^iSe_6^a$ cluster units in a 1:1 ratio. Both components are interconnected through interunit Mo—Se bonds. The cluster units are centered at Wyckoff positions 3*a* and 3*b* (point-group symmetry $\overline{3}$.). The two $Tl^I$ atoms are situated in the voids of the three-dimensional arrangement. Two of the five independent Se atoms and the Tl atoms lie on sites with 3. symmetry (Wyckoff site 6*c*).

## Related literature

For the crystal structure of $Tl_2Mo_9S_{11}$, see: Potel *et al.* (1980). For details of the *i*- and *a*-type ligand notation, see: Schäfer & von Schnering (1964). Ionic radii were compiled by Shannon (1976). For background to the extinction correction, see: Becker & Coppens (1974).

## Experimental

### *Crystal data*

$Tl_2Mo_9Se_{11}$
$M_r$ = 2140.8
Trigonal, $R\overline{3}$
$a$ = 9.6212 (1) Å
$c$ = 36.3316 (7) Å
$V$ = 2912.55 (7) Å$^3$
$Z$ = 6
Mo $K\alpha$ radiation
$\mu$ = 42.73 mm$^{-1}$
$T$ = 293 K
0.13 × 0.12 × 0.11 mm

### *Data collection*

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*PLATON*; Spek, 2009)
$T_{min}$ = 0.033, $T_{max}$ = 0.108
21097 measured reflections
4097 independent reflections
3156 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.087

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.092
$S$ = 1.37
4097 reflections
69 parameters
$\Delta\rho_{max}$ = 3.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.89 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Tl1—Tl2$^{i}$ | 3.5164 (7) | Mo1—Mo1$^{x}$ | 2.7609 (6) |
| Tl1—Se2 | 4.3543 (6) | Mo1—Mo2$^{viii}$ | 3.4239 (8) |
| Tl1—Se2$^{ii}$ | 4.3543 (7) | Mo1—Se1 | 2.5540 (8) |
| Tl1—Se2$^{iii}$ | 4.3543 (7) | Mo1—Se1$^{x}$ | 2.6143 (8) |
| Tl1—Se3 | 3.5840 (6) | Mo1—Se1$^{xiii}$ | 2.5757 (6) |
| Tl1—Se3$^{ii}$ | 3.5840 (5) | Mo1—Se2 | 2.6247 (8) |
| Tl1—Se3$^{iii}$ | 3.5840 (8) | Mo1—Se4 | 2.5269 (8) |
| Tl1—Se3$^{iv}$ | 3.4547 (6) | Mo2—Mo2$^{ix}$ | 2.6382 (5) |
| Tl1—Se3$^{v}$ | 3.4547 (8) | Mo2—Mo3 | 2.7397 (7) |
| Tl1—Se3$^{vi}$ | 3.4547 (5) | Mo2—Mo3$^{viii}$ | 2.7901 (7) |
| Tl1—Se4$^{vii}$ | 3.0737 (10) | Mo2—Se1$^{i}$ | 2.6597 (6) |
| Tl2—Se1 | 3.4032 (7) | Mo2—Se2 | 2.6034 (9) |
| Tl2—Se1$^{viii}$ | 3.4032 (6) | Mo2—Se2$^{ix}$ | 2.6124 (10) |
| Tl2—Se1$^{ix}$ | 3.4032 (8) | Mo2—Se3 | 2.6721 (6) |
| Tl2—Se2$^{i}$ | 3.1441 (4) | Mo2—Se5 | 2.5129 (8) |
| Tl2—Se2$^{x}$ | 3.1441 (7) | Mo3—Mo3$^{ix}$ | 2.6780 (7) |
| Tl2—Se2$^{xi}$ | 3.1441 (7) | Mo3—Mo3$^{xiv}$ | 2.6796 (6) |
| Tl2—Se3$^{i}$ | 4.2446 (7) | Mo3—Se2$^{ix}$ | 2.5634 (8) |
| Tl2—Se3$^{x}$ | 4.2446 (6) | Mo3—Se3 | 2.6090 (6) |
| Tl2—Se3$^{xi}$ | 4.2446 (8) | Mo3—Se3$^{ix}$ | 2.6112 (6) |
| Tl2—Se5 | 3.0483 (9) | Mo3—Se3$^{xiv}$ | 2.7025 (8) |
| Mo1—Mo1$^{xii}$ | 2.6897 (7) | | |

Symmetry codes: (i) $-x+\frac{1}{3}, -y+\frac{2}{3}, -z+\frac{2}{3}$; (ii) $-y+1, x-y+1, z$; (iii) $-x+y, -x+1, z$; (iv) $-x+1, -y+1, -z+1$; (v) $y, -x+y+1, -z+1$; (vi) $x-y, x, -z+1$; (vii) $-x, -y+1, -z+1$; (viii) $-y, x-y, z$; (ix) $-x+y, -x, z$; (x) $y-\frac{2}{3}, -x+y-\frac{1}{3}, -z+\frac{2}{3}$; (xi) $x-y+\frac{1}{3}, x-\frac{1}{3}, -z+\frac{2}{3}$; (xii) $-x+y-1, -x, z$; (xiii) $x-y+\frac{1}{3}, x+\frac{2}{3}, -z+\frac{2}{3}$; (xiv) $y, -x+y, -z+1$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *COLLECT*; data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *JANA2006*.

Intensity data were collected at the 'Centre de diffractométrie de l'Université de Rennes I' (www.cdifx.univ-rennes1.fr).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2368).

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# supporting information

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## $Tl_2Mo_9Se_{11}$

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### S1. Comment

Potel *et al.* (1980) reported the crystal structure of $Tl_2Mo_9S_{11}$ that was the first compound containing a transition metal cluster with a nuclearity higher than 9, namely the trioctahedral $Mo_{12}$ cluster. The latter cluster, which results from the uniaxial face-sharing of three $Mo_6$ octahedra, coexists with the octahedral $Mo_6$ cluster in equal proportion. We present here the crystal structure of the isotypic selenide, $Tl_2Mo_9Se_{11}$.

The Mo—Se framework of $Tl_2Mo_9Se_{11}$ consists of an equal mixture of $Mo_6Se^i_8Se^a_6$ and $Mo_{12}Se^i_{14}Se^a_6$ cluster units interconnected through Mo—Se bonds (Fig.1 and 2). Details of the *i*- and *a*-type ligand notation were reported by Schäfer & von Schnering (1964). The first unit can be described as an $Mo_6$ octahedron surrounded by 8 face-capping inner $Se^i$ and 6 apical $Se^a$ ligands. The $Mo_{12}$ core of the second unit results from the face sharing of 3 octahedral $Mo_6$ clusters. The $Mo_{12}$ cluster is surrounded by 14 $Se^i$ atoms capping the faces of the bioctahedron and 6 apical $Se^a$ ligands above the ending Mo atoms. The $Mo_6Se^i_8Se^a_6$ and $Mo_{12}Se^i_{14}Se^a_6$ units are centered at 3*a* and 3*b* positions and have point-group symmetry $\bar{3}$. The Mo—Mo distances within the $Mo_6$ clusters are 2.6897 (7) Å for the intra-triangle distances (distances within the $Mo_3$ triangles formed by the Mo1 atoms related through the threefold axis) and 2.7609 (6) Å for the inter-triangle distances. In the sulfide, the two later values are slightly larger, *viz*. 2.693 (1) and 2.780 (5) Å. The Mo—Mo distances within the $Mo_{12}$ clusters are 2.6382 (5) and 2.6780 (7) Å for the distances in the triangles formed by the Mo2 and Mo3 atoms, respectively. In $Tl_2Mo_9S_{11}$, the corresponding distances are equal to 2.658 (1) and 2.688 (1) Å, respectively. The distances between the triangles formed by the Mo2 and Mo3 atoms are 2.7397 (7) and 2.7901 (7) Å and those between the $Mo3_3$ triangles, 2.6796 (6) Å. The average Mo—Mo distance within the $Mo_{12}$ cluster is similar in $Tl_2Mo_9S_{11}$ and $Tl_2Mo_9Se_{11}$ and amounts to 2.705 Å. The Se atoms bridge either one (Se1, Se2, Se4 and Se5) or two (Se3) Mo triangular faces of the clusters. Moreover, the Se1 and Se2 atoms are linked to a Mo atom of a neighboring cluster. The Mo—Se bond distances range from 2.5269 (8) to 2.6247 (8) Å within the $Mo_6Se^i_8Se^a_6$ unit and from 2.5129 (8) to 2.7025 (8) Å within the $Mo_{12}Se^i_{14}Se^a_6$ ubit. Each $Mo_{12}Se^i_{14}Se^a_6$ unit is interconnected to 6 $Mo_6Se^i_8Se^a_6$ units (and *vice versa*) *via* Mo2—Se1 bonds (respectively Mo1—Se2) to form the three-dimensional Mo—Se framework, the overall connectivity formula of which is $Mo_{12}Se^i_8Se^i$-$a_{6/2}Se^a$-$i_{6/2}$, $Mo_6Se^i_2Se^i$-$a_{6/2}Se^a$-$i_{6/2}$. It results from this arrangement that the shortest intercluster Mo1—Mo2 distance between the $Mo_6$ and $Mo_{12}$ clusters is 3.4239 (8) Å compared to 3.217 (1) in $Tl_2Mo_9S_{11}$, indicating only weak metal-metal interaction. The Tl atoms occupy large voids delimited by four $Mo_6Se^i_8Se^a_6$ units and four $Mo_{12}Se^i_{14}Se^a_6$ units. The Tl1 and Tl2 cations have a very similar environment which consists of seven Se atoms as nearest neighbors with Tl—Se distances in the ranges 3.0737 (10) - 3.5840 (6) Å and 3.0483 (9) - 3.4032 (6) Å for the Tl1 and Tl2 sites, respectively. These seven Se atoms form a monocapped octahedron compressed along the threefold axis. Three additional Se atoms at 4.3543 (6) and 4.2446 (6) Å from Tl1 and Tl2, respectively, are also observed (Figure 3). The average Tl—Se values are 3.72 and 3.54 Å for the Tl1 and Tl2 sites, respectively. Values of 3.57 and 3.68 Å are expected from the sum of the ionic radii for $Se^{2-}$ and $Tl^+$ for coordination numbers 8 and 12 (Shannon, 1976).

## S2. Experimental

Single crystals of $Tl_2Mo_9Se_{11}$ were prepared from a mixture of $MoSe_2$, TlSe and Mo with the nominal composition $Tl_2Mo_{12}Se_{14}$. Before use, Mo powder was reduced under $H_2$ flowing gas at 1273 K during ten hours in order to eliminate any trace of oxygen. The binaries $MoSe_2$ and TlSe were obtained by heating stoichiometric mixtures of the elements in sealed evacuated silica tubes during about 2 days at 1073 and 573 K, respectively. All handlings of materials were done in an argon-filled glove box. The initial mixture (*ca* 5 g) was cold pressed and loaded into a molybdenum crucible, which was sealed under a low argon pressure using an arc welding system. The charge was heated at the rate of 300 K/h up to 1773 K, the temperature which was held for 48 h, then cooled at 100 K/h down to 1373 K and finally furnace cooled.

## S3. Refinement

The highest peak and the deepest hole in the final Fourier map are at 1.67 and 0.83 Å from Tl1 and Se5, respectively.

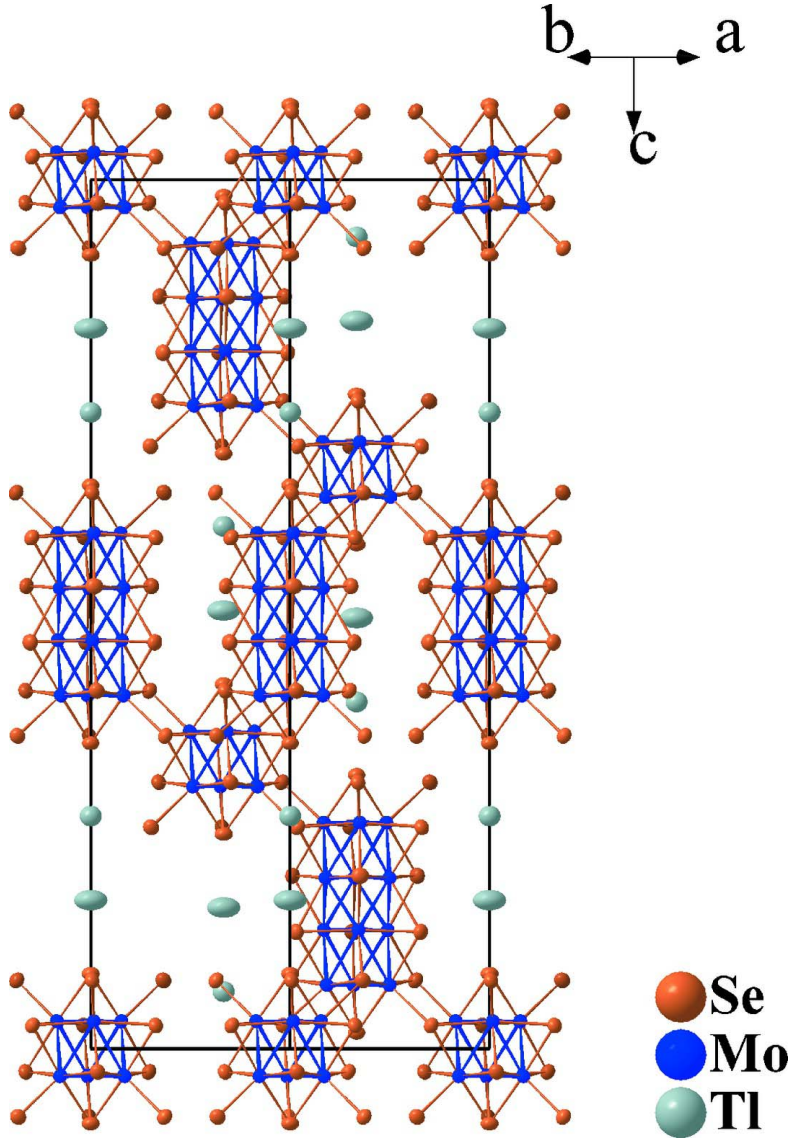


**Figure 1**

View of $Tl_2Mo_9Se_{11}$ along [110].

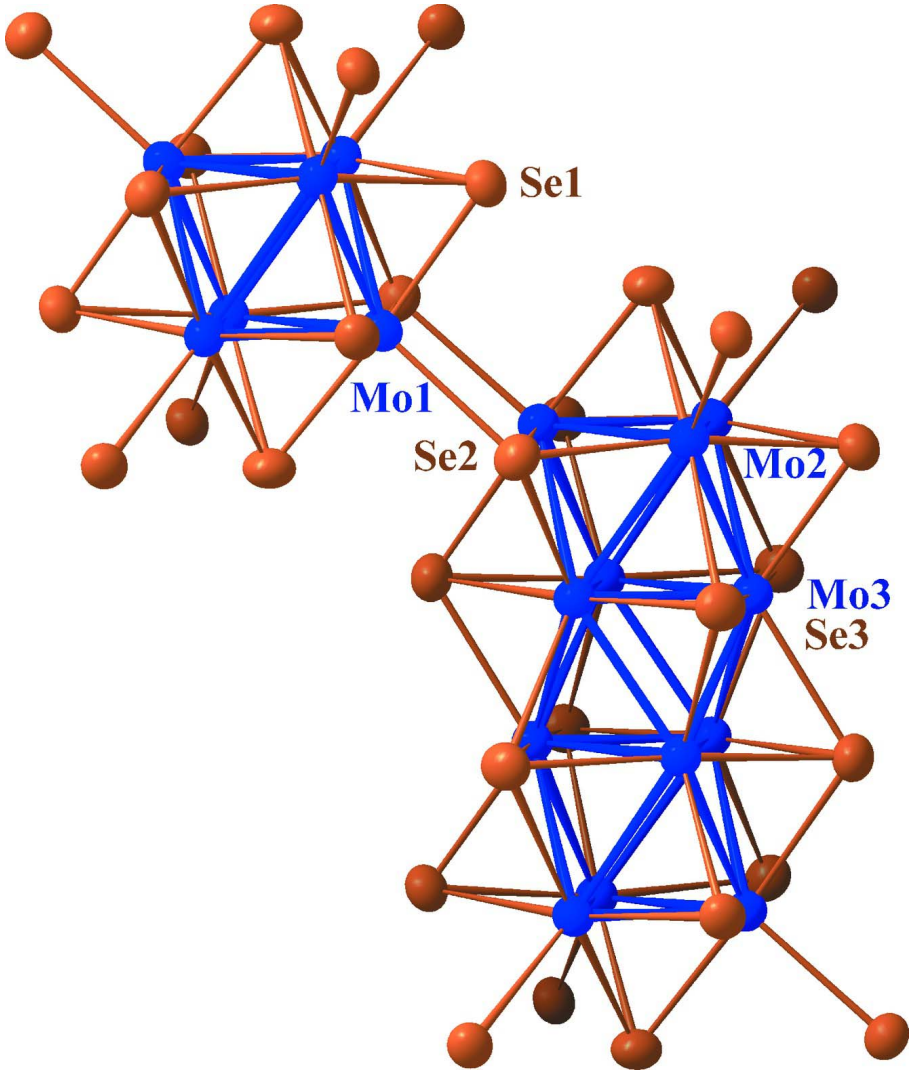


**Figure 2**

Plot showing the atom-numbering scheme and the linkage of the $Mo_{12}Se_{14}Se_6$ and $Mo_6Se_8Se_6$ cluster units. Displacement ellipsoids are drawn at the 97% probability level. Symmetry codes are as in Table 1.

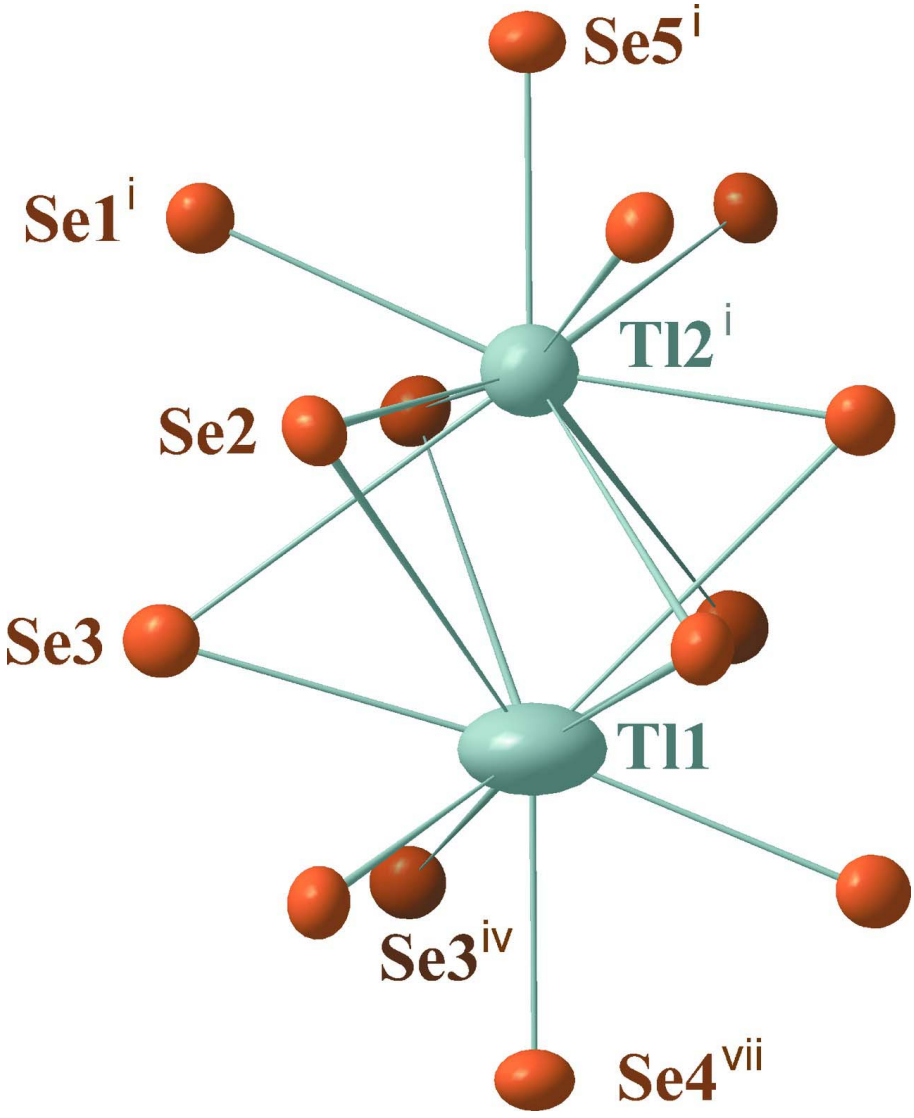


**Figure 3**

Environment of the Tl atoms. Symmetry codes are as in Table 1.

**dithallium nonamolybdenum undecaselenide**

*Crystal data*

$Tl_2Mo_9Se_{11}$
$M_r$ = 2140.8
Trigonal, $R\overline{3}$
Hall symbol: -R 3
$a$ = 9.6212 (1) Å
$c$ = 36.3316 (7) Å
$V$ = 2912.55 (7) Å$^3$
$Z$ = 6
$F$(000) = 5484
$D_x$ = 7.321 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71069 Å
Cell parameters from 10017 reflections
$\theta$ = 1–40.3°
$\mu$ = 42.73 mm$^{-1}$
$T$ = 293 K
Irregular block, black
0.13 × 0.12 × 0.11 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\varphi$– and $\omega$–scans
Absorption correction: multi-scan (*PLATON*; Spek, 2009)

$T_{min}$ = 0.033, $T_{max}$ = 0.108
21097 measured reflections
4097 independent reflections
3156 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.087
$\theta_{max}$ = 40.2°, $\theta_{min}$ = 1.7°
$h$ = −16→17
$k$ = −16→17
$l$ = −58→66

*Refinement*

Refinement on $F^2$
$R[F > 3\sigma(F)]$ = 0.043
$wR(F)$ = 0.092
$S$ = 1.37
4097 reflections
69 parameters
0 restraints
0 constraints

Weighting scheme based on measured s.u.'s $w = 1/[\sigma^2(I) + 0.0004I^2]$
$(\Delta/\sigma)_{max}$ = 0.033
$\Delta\rho_{max}$ = 3.92 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.89 e Å$^{-3}$
Extinction correction: B-C type 1 Gaussian isotropic (Becker & Coppens, 1974)
Extinction coefficient: 2320 (40)

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Tl1 | 0.333333 | 0.666667 | 0.495781 (14) | 0.04933 (17) |
| Tl2 | 0 | 0 | 0.267672 (12) | 0.02611 (11) |
| Mo1 | −0.18022 (5) | 0.31787 (5) | 0.364749 (12) | 0.01129 (13) |
| Mo2 | 0.16529 (5) | 0.15027 (5) | 0.406587 (12) | 0.01120 (13) |
| Mo3 | 0.15606 (5) | −0.00891 (5) | 0.469882 (12) | 0.01087 (13) |
| Se1 | −0.04118 (6) | 0.29911 (6) | 0.306626 (15) | 0.01295 (17) |
| Se2 | 0.03067 (6) | 0.32633 (6) | 0.411871 (15) | 0.01342 (17) |
| Se3 | 0.32150 (6) | 0.30388 (6) | 0.467628 (15) | 0.01463 (17) |
| Se4 | −0.333333 | 0.333333 | 0.41962 (2) | 0.01559 (19) |
| Se5 | 0 | 0 | 0.35157 (2) | 0.01474 (19) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Tl1 | 0.0620 (2) | 0.0620 (2) | 0.0239 (2) | 0.03102 (12) | 0 | 0 |
| Tl2 | 0.02704 (13) | 0.02704 (13) | 0.0242 (2) | 0.01352 (7) | 0 | 0 |
| Mo1 | 0.01119 (17) | 0.01064 (17) | 0.01168 (17) | 0.00518 (13) | 0.00061 (13) | −0.00028 (13) |
| Mo2 | 0.01129 (17) | 0.01096 (17) | 0.01107 (17) | 0.00535 (14) | 0.00023 (13) | 0.00051 (13) |
| Mo3 | 0.01081 (16) | 0.01111 (16) | 0.01077 (17) | 0.00553 (13) | 0.00040 (13) | 0.00014 (13) |
| Se1 | 0.0120 (2) | 0.0136 (2) | 0.0140 (2) | 0.00691 (17) | 0.00193 (16) | 0.00090 (16) |
| Se2 | 0.0145 (2) | 0.0121 (2) | 0.0140 (2) | 0.00685 (17) | −0.00087 (17) | 0.00125 (16) |
| Se3 | 0.0121 (2) | 0.0135 (2) | 0.0151 (2) | 0.00408 (17) | 0.00057 (17) | 0.00032 (17) |
| Se4 | 0.0181 (2) | 0.0181 (2) | 0.0106 (3) | 0.00905 (12) | 0 | 0 |
| Se5 | 0.0167 (2) | 0.0167 (2) | 0.0108 (3) | 0.00835 (11) | 0 | 0 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Tl1—Tl2$^{i}$ | 3.5164 (7) | Mo1—Mo1$^{xiv}$ | 2.7609 (7) |
| Tl1—Se2 | 4.3543 (6) | Mo1—Mo2$^{viii}$ | 3.4239 (8) |
| Tl1—Se2$^{ii}$ | 4.3543 (7) | Mo1—Se1 | 2.5540 (8) |
| Tl1—Se2$^{iii}$ | 4.3543 (7) | Mo1—Se1$^{x}$ | 2.6143 (8) |
| Tl1—Se3 | 3.5840 (6) | Mo1—Se1$^{xiv}$ | 2.5757 (6) |
| Tl1—Se3$^{ii}$ | 3.5840 (5) | Mo1—Se2 | 2.6247 (8) |
| Tl1—Se3$^{iii}$ | 3.5840 (8) | Mo1—Se4 | 2.5269 (8) |
| Tl1—Se3$^{iv}$ | 3.4547 (6) | Mo2—Mo2$^{viii}$ | 2.6382 (6) |
| Tl1—Se3$^{v}$ | 3.4547 (8) | Mo2—Mo2$^{ix}$ | 2.6382 (5) |
| Tl1—Se3$^{vi}$ | 3.4547 (5) | Mo2—Mo3 | 2.7397 (7) |
| Tl1—Se4$^{vii}$ | 3.0737 (10) | Mo2—Mo3$^{viii}$ | 2.7901 (7) |
| Tl2—Se1 | 3.4032 (7) | Mo2—Se1$^{i}$ | 2.6597 (6) |
| Tl2—Se1$^{viii}$ | 3.4032 (6) | Mo2—Se2 | 2.6034 (9) |
| Tl2—Se1$^{ix}$ | 3.4032 (8) | Mo2—Se2$^{ix}$ | 2.6124 (10) |
| Tl2—Se2$^{i}$ | 3.1441 (4) | Mo2—Se3 | 2.6721 (6) |
| Tl2—Se2$^{x}$ | 3.1441 (7) | Mo2—Se5 | 2.5129 (8) |
| Tl2—Se2$^{xi}$ | 3.1441 (7) | Mo3—Mo3$^{viii}$ | 2.6780 (9) |
| Tl2—Se3$^{i}$ | 4.2446 (7) | Mo3—Mo3$^{ix}$ | 2.6780 (7) |
| Tl2—Se3$^{x}$ | 4.2446 (6) | Mo3—Mo3$^{xv}$ | 2.6796 (6) |
| Tl2—Se3$^{xi}$ | 4.2446 (8) | Mo3—Mo3$^{vi}$ | 2.6796 (7) |
| Tl2—Se5 | 3.0483 (9) | Mo3—Se2$^{ix}$ | 2.5634 (8) |
| Mo1—Mo1$^{xii}$ | 2.6897 (9) | Mo3—Se3 | 2.6090 (6) |
| Mo1—Mo1$^{xiii}$ | 2.6897 (7) | Mo3—Se3$^{ix}$ | 2.6112 (6) |
| Mo1—Mo1$^{x}$ | 2.7609 (6) | Mo3—Se3$^{xv}$ | 2.7025 (8) |
| | | | |
| Mo1$^{xii}$—Mo1—Mo1$^{xiii}$ | 60.000 (18) | Mo2—Mo3—Mo3$^{ix}$ | 90.11 (2) |
| Mo1$^{xii}$—Mo1—Mo1$^{x}$ | 90 | Mo2—Mo3—Mo3$^{xv}$ | 147.49 (3) |
| Mo1$^{xii}$—Mo1—Mo1$^{xiv}$ | 60.85 (2) | Mo2—Mo3—Mo3$^{vi}$ | 111.83 (2) |
| Mo1$^{xiii}$—Mo1—Mo1$^{x}$ | 60.849 (16) | Mo2$^{ix}$—Mo3—Mo3$^{viii}$ | 89.04 (2) |
| Mo1$^{xiii}$—Mo1—Mo1$^{xiv}$ | 90 | Mo2$^{ix}$—Mo3—Mo3$^{ix}$ | 60.094 (17) |
| Mo1$^{x}$—Mo1—Mo1$^{xiv}$ | 58.302 (17) | Mo2$^{ix}$—Mo3—Mo3$^{xv}$ | 110.275 (17) |
| Mo2$^{viii}$—Mo2—Mo2$^{ix}$ | 60.00 (2) | Mo2$^{ix}$—Mo3—Mo3$^{vi}$ | 145.90 (3) |
| Mo2$^{viii}$—Mo2—Mo3 | 90.953 (18) | Mo3$^{viii}$—Mo3—Mo3$^{ix}$ | 60.000 (18) |
| Mo2$^{viii}$—Mo2—Mo3$^{viii}$ | 60.546 (16) | Mo3$^{viii}$—Mo3—Mo3$^{xv}$ | 90 |
| Mo2$^{ix}$—Mo2—Mo3 | 62.472 (16) | Mo3$^{viii}$—Mo3—Mo3$^{vi}$ | 60.02 (2) |
| Mo2$^{ix}$—Mo2—Mo3$^{viii}$ | 89.850 (19) | Mo3$^{ix}$—Mo3—Mo3$^{xv}$ | 60.019 (16) |
| Mo3—Mo2—Mo3$^{viii}$ | 57.92 (2) | Mo3$^{ix}$—Mo3—Mo3$^{vi}$ | 90 |
| Mo2—Mo3—Mo2$^{ix}$ | 56.983 (15) | Mo3$^{xv}$—Mo3—Mo3$^{vi}$ | 59.962 (18) |
| Mo2—Mo3—Mo3$^{viii}$ | 61.982 (19) | | |

Symmetry codes: (i) −*x*+1/3, −*y*+2/3, −*z*+2/3; (ii) −*y*+1, *x*−*y*+1, *z*; (iii) −*x*+*y*, −*x*+1, *z*; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *y*, −*x*+*y*+1, −*z*+1; (vi) *x*−*y*, *x*, −*z*+1; (vii) −*x*, −*y*+1, −*z*+1; (viii) −*y*, *x*−*y*, *z*; (ix) −*x*+*y*, −*x*, *z*; (x) *y*−2/3, −*x*+*y*−1/3, −*z*+2/3; (xi) *x*−*y*+1/3, *x*−1/3, −*z*+2/3; (xii) −*y*, *x*−*y*+1, *z*; (xiii) −*x*+*y*−1, −*x*, *z*; (xiv) *x*−*y*+1/3, *x*+2/3, −*z*+2/3; (xv) *y*, −*x*+*y*, −*z*+1.