V1.42In1.83Mo15Se19
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The structure of the title compound, vanadium indium pentadecamolybdenum nonadecasilenide, \( \text{V}_{1.42}\text{In}_{1.83}\text{Mo}_{15}\text{Se}_{19} \), is isotypic with \( \text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19} \) [Grüttner et al. (1979). Acta Cryst. B35, 285–292]. It is characterized by two cluster units \( \text{Mo}_6\text{Se}_{11} \) and \( \text{Mo}_6\text{Se}_{11} \) (where \( i \) represents inner and \( a \) apical atoms) that are present in a 1:1 ratio. The cluster units are centered at Wyckoff positions 2\( a \) and 2\( c \) and have point-symmetry 3\( a \) and 6\( i \), respectively. The clusters are interconnected through additional Mo–Se bonds. In the title compound, the \( V^{5+} \) cations replace the trivalent indium atoms present in \( \text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19} \), and a deficiency is observed on the monovalent indium site. One Mo, one Se and the V atom are situated on mirror planes, and two other Se atoms and the In atom are situated on threefold rotation axes.

Related literature

For previous reports on the crystal structure of \( \text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19} \) compounds, see: Grüttner et al. (1979). For physical properties of this type of compound, see: Seeber et al. (1979). The crystal structures of the substituted compounds \( \text{Ho}_{0.76}\text{In}_{1.68}\text{Mo}_{15}\text{Se}_{19} \) and \( \text{In}_{0.87}\text{K}_{2.01}\text{Mo}_{15}\text{Se}_{19} \) were reported by Salloum et al. (2006; 2007). For details of the \( i \)- and \( a \)-type ligand notation, see: Schäfer & von Schnerring (1964).

Experimental

Crystal data

\( \text{V}_{1.42}\text{In}_{1.83}\text{Mo}_{15}\text{Se}_{19} \)

- \( M_r = 3221.80 \)
- Hexagonal, \( P6_3/m \)
- \( a = 9.7361 \) (1) \( \AA \)
- \( c = 19.3090 \) (4) \( \AA \)
- \( V = 1585.11 \) (4) \( \AA^3 \)
- \( Z = 2 \)
- Mo Ka radiation
- \( \mu = 29.21 \) mm\(^{-1} \)
- \( T = 293 \) K
- \( 0.09 \times 0.07 \times 0.05 \) mm

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V$_{1.42}$In$_{1.83}$Mo$_{15}$Se$_{19}$

P. Gougeon, P. Gall, D. Salloum and M. Potel

Comment

From the point of view of crystal chemistry and physical properties, the reduced molybdenum selenides In$_3$Mo$_{15}$Se$_{19}$ (Grüttner et al., 1979) constitute an interesting family of compounds. Indeed, their crystal structure contains an equal mixture of Mo$_6$ and Mo$_9$ cluster units and the In atoms occupy two crystallographically different positions depending on their formal oxidation state of +1 or +3. Recently, we have shown that the In$^{3+}$ cation can be replaced by other trivalent cations such as Ho$^{3+}$ (Salloum et al., 2006) and the In$^+$ cation by K$^+$ (Salloum et al., 2007). Interest in these Mo cluster compounds also lies in their physical properties, because they become superconductors with high critical magnetic fields at about 4 K (Seeber et al., 1979). We present here the crystal structure of V$_{1.42}$In$_{1.83}$Mo$_{15}$Se$_{19}$ in which a 3$d$ element replaces the trivalent indium atom.

The Mo—Se framework of the title compound consists of the cluster units Mo$_6$Se$_8^{i}Se_{6}^{a}$ and Mo$_9$Se$_{11}^{i}$Se$_6^{a}$ in a 1:1 ratio (for details of the $i$- and $a$-type ligand notation, see: Schäfer & von Schnering (1964)). Both cluster units are interconnected through additional Mo—Se bonds (Figs. 1 and 2). The first unit can be described as an Mo$_6$ octahedron surrounded by eight face-capping inner Se$^{i}$ and six apical Se$^{a}$ ligands. The Mo$_9$ cluster is surrounded by 11 Se$^{i}$ atoms capping one or two faces of the bioctahedron and six Se$^{a}$ ligands above the apical Mo atoms. The Mo$_6$Se$_8^{i}Se_{6}^{a}$ and Mo$_9$Se$_{11}^{i}$Se$_6^{a}$ units are centered at Wyckoff positions 2$b$ and 2$c$ and have point-group symmetry $3$ and $6$, respectively. The Mo—Mo distances within the Mo$_6$ cluster are 2.6992 (7) Å for the distances of the Mo triangles formed by the Mo$_1$ atoms related through the threefold axis, and 2.7223 (8) Å for the distances between these triangles. The Mo—Mo distances within the Mo$_9$ clusters are 2.6474 (7) and 2.7056 (10) Å in the triangles formed by the atoms Mo$_2$ and Mo$_3$, respectively, and 2.7136 (5) and 2.7557 (5) Å for those between the Mo$_2$ and Mo$_3$ triangles. The Se atoms bridge either one (Se$_1$, Se$_2$, Se$_4$ and Se$_5$) or two (Se$_3$) triangular faces of the Mo clusters. Moreover, atoms Se$_1$ and Se$_2$ are linked to an Mo atom of a neighboring cluster. The Mo—Se bond lengths range from 2.5467 (7) to 2.6378 (7) Å within the Mo$_6$Se$_8^{i}Se_{6}^{a}$ unit, and from 2.5259 (8) to 2.6966 (6) Å within the Mo$_9$Se$_{11}^{i}$Se$_6^{a}$ unit. Each Mo$_9$Se$_{11}^{i}$Se$_6^{a}$ cluster is interconnected by six Mo$_6$Se$_8^{i}Se_{6}^{a}$ units (and vice versa) via Mo$_2$—Se$_1$ bonds (and Mo$_1$—Se$_2$ bonds, respectively), forming the three-dimensional Mo—Se framework, the connectivity formula of which is Mo$_9$Se$_{8}^{i}Se_{6}^{a}$, Mo$_6$Se$_8^{i}Se_{6}^{a}$, Mo$_9$Se$_{11}^{i}$Se$_6^{a}$, Mo$_6$Se$_8^{i}Se_{6}^{a}$, and Mo$_9$Se$_{11}^{i}$Se$_6^{a}$. It results from this arrangement that the shortest intercluster Mo$_1$—Mo$_2$ distance is 3.4216 (6) Å, indicating only weak metal—metal interaction. The In$^+$ cations are surrounded by seven Se atoms forming a distorted tricapped tetrahedron, as is the case in In$_2$9Mo$_{15}$Se$_{19}$. The Se$_5$ and Se$_2$ atoms forming the tetrahedron are at 3.0759 (15) and 3.1221 (5) Å from the In atom, and the capping Se$_1$ atoms are at 3.4904 (7) Å. The V$^{3+}$ cations, as the In$^{3+}$ cations in the In$_3$Mo$_{15}$Se$_{19}$ compounds, occupy partially at 47.4 (6)% a triangular group of distorted octahedral cavities, which are formed by two Mo$_6$Se$_8^{i}Se_{6}^{a}$ and three Mo$_9$Se$_{11}^{i}$Se$_6^{a}$ units, around the threefold rotation axis. The V—Se distances are in the 2.510 (2) - 2.831 (3) Å range.
supplementary materials

Experimental

Single crystals of $V_{1.42}In_{1.83}Mo_{15}Se_{19}$ were prepared from a mixture of $V_2Se_3$, $MoSe_2$, InSe and Mo with a nominal composition $V_{1.5}In_2Mo_{15}Se_{19}$. 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 $V_2Se_3$, $MoSe_2$, InSe were obtained by heating stoichoetric mixtures of the elements in sealed evacuated silica tubes during about 2 days. 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 hours, then cooled at 100 K/h down to 1373 K and finally furnace cooled.

Refinement

The highest peak and the deepest hole are located 1.56 Å and 0.66 Å from Mo3, respectively. Refinement of the occupancy factors of the V and In atoms led to the final composition $V_{1.42(2)}In_{1.832(8)}Mo_{15}Se_{19}$.

Figures

Fig. 1. View of $V_{1.42}In_{1.83}Mo_{15}Se_{19}$ along [110]. Displacement ellipsoids are drawn at the 97% probability level.

Fig. 2. Plot showing the atom-numbering scheme and the interunit linkage of the $Mo_9Se_{11}Se_6$ and $Mo_6Se_9Se_6$ cluster units. Displacement ellipsoids are drawn at the 97% probability level.

vanadium indium pentadecamolybdenum nonadecaselenide

Crystal data

| Formula          | Density $D_x$ [Mg m$^{-3}$] |
|------------------|-----------------------------|
| $V_{1.42}In_{1.83}Mo_{15}Se_{19}$ | 6.750 |

| Molar mass $M_r$  | Radiation $\lambda$, $\mu$ [Å, mm$^{-1}$] |
|-------------------|-------------------------------------------|
| 3221.80           | Mo $K_a$, 0.71069 Å, 29.21 mm$^{-1}$       |

| Crystal system    | Space group   |
|-------------------|---------------|
| Hexagonal, $P6_3/m$|               |

| Hall symbol       | Number of reflections |
|-------------------|-----------------------|
| -$P6_3$           | 26495                 |

| Cell parameters   | |
|-------------------|-----------------|
| $a$ = 9.7361 (1) Å | $\theta = 2.6-35.0^\circ$ |
| $c$ = 19.3090 (4) Å | $\mu = 29.21$ mm$^{-1}$ |

| Temperature $T$   | |
|-------------------|-----------------|
| 293 K             | $T = 293$ K     |
$V = 1585.11\ (4) \text{ Å}^3$

Irregular block, black

$Z = 2$

$0.09 \times 0.07 \times 0.05 \text{ mm}$

**Data collection**

Nonius KappaCCD
diffractometer

2390 independent reflections

Radiation source: fine-focus sealed tube

graphite

$R_{int} = 0.093$

$\varphi$ scans ($\chi = 0$) + additional $\omega$ scans

$\theta_{max} = 35.0^\circ$, $\theta_{min} = 2.6^\circ$

Absorption correction: analytical
(de Meulenaar & Tompa, 1965)

$h = -15\rightarrow 15$

$T_{min} = 0.161$, $T_{max} = 0.329$

$27560$ measured reflections

**Refinement**

Refinement on $F^2$

Primary atom site location: structure-invariant direct methods

Least-squares matrix: full Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.087$

$S = 1.08$

2390 reflections

67 parameters

0 restraints

Extinction correction: SHELXL97 (Sheldrick, 2008), $F^c = kF[1 + 0.001xF^2\lambda^2/\sin(2\theta)]^{1/4}$

Extinction coefficient: 0.00025 (5)

**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 ($\text{Å}^2$)**

|     | $x$     | $y$     | $z$     | $U_{iso}^{eq}$ | Occ. (<1) |
|-----|---------|---------|---------|----------------|-----------|
| Mo1 | 0.16776 (5) | 0.01669 (5) | 0.55780 (2) | 0.00914 (10) |           |
| Mo2 | 0.68407 (5) | 0.18577 (5) | 0.63317 (2) | 0.00965 (10) |           |
| Mo3 | 0.51292 (7) | 0.16694 (7) | 0.7500   | 0.00868 (11) |           |
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| \( Se_1 \)   | 0.03647 (6)   | -0.28702 (6) | 0.55134 (3) | 0.01070 (11) |
| \( Se_2 \)   | 0.37798 (6)   | 0.00665 (6)  | 0.64065 (3) | 0.01233 (12) |
| \( Se_3 \)   | 0.34594 (8)   | 0.30753 (9)  | 0.7500      | 0.01280 (15) |
| \( Se_4 \)   | 0.0000        | 0.0000       | 0.66221 (5) | 0.01643 (19) |
| \( Se_5 \)   | 0.6667        | 0.3333       | 0.52902 (5) | 0.01225 (17) |
| \( In_1 \)   | 0.6667        | 0.3333       | 0.36972 (6) | 0.0374 (4)   |
| \( V_1 \)    | -0.2026 (4)   | -0.1744 (3)  | 0.7500      | 0.916 (4)    |

Atomic displacement parameters (Å\(^2\))

|        | \( U_{11} \) | \( U_{22} \) | \( U_{33} \) | \( U_{12} \) | \( U_{13} \) | \( U_{23} \) |
|--------|--------------|--------------|--------------|--------------|--------------|--------------|
| \( Mo_1 \) | 0.00996 (18) | 0.00853 (18) | 0.0089 (2)   | 0.00456 (15) | 0.00070 (14) | -0.00012 (14) |
| \( Mo_2 \) | 0.00995 (18) | 0.00993 (18) | 0.0089 (2)   | 0.00488 (15) | 0.00013 (14) | -0.00037 (14) |
| \( Mo_3 \) | 0.0096 (2)   | 0.0099 (3)   | 0.0071 (3)   | 0.0053 (2)   | 0.0000       | 0.0000       |
| \( Se_1 \) | 0.0110 (2)   | 0.0097 (2)   | 0.0116 (2)   | 0.00543 (19) | 0.00107 (17) | 0.00229 (17) |
| \( Se_2 \) | 0.0115 (2)   | 0.0119 (2)   | 0.0138 (3)   | 0.00598 (18) | -0.00305 (18) | -0.00208 (18) |
| \( Se_3 \) | 0.0121 (3)   | 0.0158 (3)   | 0.0117 (3)   | 0.0079 (3)   | 0.0000       | 0.0000       |
| \( Se_4 \) | 0.0203 (3)   | 0.0203 (3)   | 0.0086 (4)   | 0.01016 (14) | 0.0000       | 0.0000       |
| \( Se_5 \) | 0.0142 (2)   | 0.0142 (2)   | 0.0083 (4)   | 0.00712 (12) | 0.0000       | 0.0000       |
| \( In_1 \) | 0.0345 (4)   | 0.0345 (4)   | 0.0431 (7)   | 0.0172 (2)   | 0.0000       | 0.0000       |
| \( V_1 \)  | 0.0216 (16)  | 0.0095 (13)  | 0.0165 (16)  | 0.0038 (11)  | 0.0000       | 0.0000       |

Geometric parameters (Å, °)

| \( Mo_2—Se_5 \) | 2.5259 (8) | \( Mo_3—Mo_3^{ii} \) | 2.7056 (10) |
| \( Mo_2—Se_2 \) | 2.5974 (6) | \( Mo_3—Mo_3^{i} \) | 2.7056 (10) |
| \( Mo_2—Se_2^{i} \) | 2.6290 (6) | \( Mo_3—Mo_2^{ix} \) | 2.7136 (5)  |
| \( Mo_2—Mo_2^{i} \) | 2.6474 (7) | \( Mo_3—Mo_2^{ii} \) | 2.7136 (5)  |
| \( Mo_2—Mo_2^{ii} \) | 2.6474 (7) | \( Mo_3—Mo_2^{viii} \) | 2.7557 (5)  |
| \( Mo_2—Se_1^{iii} \) | 2.6504 (6) | \( In_1—Se_5 \) | 3.0759 (15) |
| \( Mo_2—Se_3^{i} \) | 2.6966 (6) | \( In_1—Se_2^{x} \) | 3.1221 (5)  |
| \( Mo_2—Mo_3^{i} \) | 2.7136 (5) | \( In_1—Se_2^{xi} \) | 3.1221 (5)  |
| \( Mo_2—Mo_3 \) | 2.7557 (5) | \( In_1—Se_2^{iv} \) | 3.1221 (5)  |
| \( Mo_1—Se_1^{iv} \) | 2.5467 (7) | \( In_1—Se_1^{x} \) | 3.4904 (7)  |
| \( Mo_1—Se_4 \) | 2.5481 (8) | \( In_1—Se_1^{xi} \) | 3.4904 (7)  |
| \( Mo_1—Se_1 \) | 2.5717 (6) | \( In_1—Se_1^{iv} \) | 3.4904 (7)  |
| \( Mo_1—Se_1^{v} \) | 2.6111 (6) | \( In_1—Se_3 \) | 4.2444 (9)  |
| \( Mo_1—Se_2 \) | 2.6378 (7) | \( In_1—Se_3^{xii} \) | 4.2444 (9)  |
| \( Mo_1—Mo_1^{i} \) | 2.6992 (7) | \( In_1—Se_3^{xiii} \) | 4.2444 (9)  |
| \( Mo_1—Mo_1^{v} \) | 2.6992 (7) | \( V_1—Se_4 \) | 2.510 (2)   |
| \( Mo_1—Mo_1^{vii} \) | 2.7223 (8) | \( V_1—Se_4^{viii} \) | 2.510 (2)   |
| \( Mo_1—Mo_1^{iv} \) | 2.7223 (8) | \( V_1—Se_3^{v} \) | 2.730 (3)   |
| \( Mo_3—Se_2 \) | 2.5631 (6) | \( V_1—Se_2^{vi} \) | 2.7981 (18) |
| \( Mo_3—Se_2^{viii} \) | 2.5631 (6) | \( V_1—Se_2^{xvii} \) | 2.7981 (18) |
| \( Mo_3—Se_3 \) | 2.5965 (9) | \( V_1—Se_3^{vi} \) | 2.831 (3)   |
| \( Mo_3—Se_3^{v} \) | 2.5965 (9) | \( V_1—Se_3^{vi} \) | 2.831 (3)   |
| Bond                  | Distance (Å) | Error (Å) |
|-----------------------|--------------|-----------|
| Mo3—Se3^i             | 2.6095       | (9)       |
| Se5—Mo2—Se2           | 92.603       | (17)      |
| Se5—Mo2—Se2^i         | 91.858       | (17)      |
| Se2—Mo2—Se2^i         | 173.59       | (3)       |
| Se5—Mo2—Mo2^i         | 58.396       | (13)      |
| Se2—Mo2—Mo2^i         | 120.06       | (2)       |
| Se5—Mo2—Mo2^ii        | 58.978       | (19)      |
| Se2—Mo2—Mo2^ii        | 58.396       | (13)      |
| Se2^i—Mo2—Mo2^ii      | 60.16        | (2)       |
| Mo2^i—Mo2—Se1^iii     | 118.878      | (19)      |
| Mo2^i—Mo2—Se1^ii      | 60.0         |           |
| Se5—Mo2—Se1^iii       | 90.42        | (2)       |
| Se2—Mo2—Se1^iii       | 86.03        | (2)       |
| Se2^i—Mo2—Se1^ii      | 98.54        | (2)       |
| Mo2^i—Mo2—Se1^ii      | 137.757      | (18)      |
| Mo2^ii—Mo2—Se1^iii    | 129.74       | (2)       |
| Se5—Mo2—Mo3^i         | 175.68       | (2)       |
| Se2—Mo2—Se3^i         | 85.76        | (2)       |
| Se2^i—Mo2—Se3^i       | 89.46        | (2)       |
| Mo2^i—Mo2—Se3^i       | 119.150      | (18)      |
| Mo2^ii—Mo2—Se3^i      | 117.432      | (18)      |
| Se1^iii—Mo2—Se3^i     | 93.45        | (2)       |
| Se5—Mo2—Mo3^i         | 120.23       | (2)       |
| Se2—Mo2—Mo3^i         | 116.35       | (2)       |
| Se2^i—Mo2—Mo3^i       | 57.311       | (17)      |
| Mo2^i—Mo2—Mo3^i       | 61.851       | (15)      |
| Mo2^ii—Mo2—Mo3^i      | 91.063       | (14)      |
| Se1^ii—Mo2—Mo3^i      | 138.90       | (2)       |
| Se3^1—Mo2—Mo3^i       | 57.36        | (2)       |
| Se5—Mo2—Mo3            | 118.64       | (2)       |
| Se2—Mo2—Mo3            | 57.123       | (17)      |
| Se2^i—Mo2—Mo3          | 116.58       | (2)       |
| Mo2^i—Mo2—Mo3          | 90.142       | (14)      |
| Mo2^ii—Mo2—Mo3         | 60.255       | (15)      |
| Se1^iii—Mo2—Mo3       | 131.66       | (2)       |
| Se3^1—Mo2—Mo3          | 57.177       | (19)      |
| Mo3^i—Mo2—Mo3          | 59.29        | (2)       |
| Se1^iv—Mo1—Se4        | 176.34       | (2)       |
| Se1^iv—Mo1—Se1        | 88.948       | (17)      |
| Se4—Mo1—Se1            | 91.765       | (17)      |

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Se1IV—Mo1—Se1V 88.084 (17) Mo1VI—Se1—Mo2IV 81.114 (19)
Se4—Mo1—Se1V 90.859 (17) Mo3—Se2—Mo2 64.549 (18)
Se1—Mo1—Se1V 173.79 (3) Mo3—Se2—Mo2ii 63.004 (18)
Se1IV—Mo1—Se2 93.50 (2) Mo2—Se2—Mo2ii 60.86 (2)
Se4—Mo1—Se2 90.13 (2) Mo3—Se2—Mo1 130.39 (2)
Se1—Mo1—Se2 86.306 (19) Mo2—Se2—Mo1 126.33 (2)
Se1V—Mo1—Se2 99.32 (2) Mo2ii—Se2—Mo1 81.018 (19)
Se4—Mo1—Mo1iv 119.568 (17) Mo3—Se3—Mo3ii 62.62 (3)
Se1—Mo1—Se1 117.827 (19) Mo3—Se3—Mo2ix 61.649 (16)
Se1V—Mo1—Mo1vi 129.11 (2) Mo3—Se3—Mo2ii 62.551 (16)
Se2—Mo1—Mo1vi 118.595 (17) Mo3—Se3—Mo2ii 61.649 (16)
SeIV—Mo1—Mo1v 58.018 (12) Mo1—Se4—Mo1 142.763 (16)
Se1—Mo1—Mo1v 59.33 (2) Mo3—Se4—Mo1 142.763 (16)
Se1V—Mo1—Mo1v 117.827 (19) Mo2—Se5—Mo2 87.27 (7)
Se2—Mo1—Mo1v 129.11 (2) Mo2—Se5—In1 166.76 (13)
Mo1VI—Mo1—Mo1v 118.273 (15) Se4—V1—Se3 87.27 (7)
Se4—Mo1—Mo1vii 57.423 (15) Se4—V1—Se2vi 166.76 (13)
Se1—Mo1—Mo1vii 116.42 (2) Se4—V1—Se2vi 87.36 (2)
Se1V—Mo1—Mo1vii 132.182 (19) Se3V—V1—Se2vi 103.16 (8)
Se2—Mo1—Mo1vii 60.281 (10) Se4VIII—V1—Se2xiv 87.36 (2)
Mo1VI—Mo1—Mo1vii 90.0 Se4—V1—Se2xiv 166.76 (13)
Mo1V—Mo1—Mo1iv 58.31 (2) Se3V—V1—Se2xiv 103.16 (8)
Se4—Mo1—Mo1iv 118.273 (15) Se2VI—V1—Se2xiv 97.98 (8)
Se1—Mo1—Mo1iv 116.86 (2) Se4VIII—V1—Se3 85.09 (8)
Se1V—Mo1—Mo1iv 56.998 (14) Se4—V1—Se3vi 85.09 (8)
Se2—Mo1—Mo1iv 140.74 (2) Se3V—V1—Se3vi 169.63 (12)
Mo1VI—Mo1—Mo1iv 90.0 Se2VI—V1—Se3vi 83.50 (6)
Mo1V—Mo1—Mo1iv 60.281 (10) Se2VIII—V1—Se3vi 83.50 (6)
Mo1VII—Mo1—Mo1v 59.44 (2) Se4VIII—V1—Mo3vi 122.97 (8)
Mo1VIII—Mo1—Mo1v 110.93 (3) Se4—V1—Mo3vi 122.97 (8)
Mo2—Mo3—Se2viii 93.18 (2) Se3V—V1—Mo3vi 136.14 (12)
Mo2—Mo3—Se2 93.18 (2) Se2VII—V1—Mo3vi 53.80 (4)
Mo2VIII—Mo3—Se2i 88.30 (2) Se2VII—V1—Mo3vi

sup-6
| Bond                        | Bond Length (Å) | Bond Angle (°) |
|-----------------------------|-----------------|---------------|
| Se3—Mo3—Mo3\textsuperscript{ii} | 58.92 (3)       |               |
| Se3—Mo3—Mo3\textsuperscript{ii} | 118.45 (3)      |               |
| Se2—Mo3—Mo3\textsuperscript{i} | 117.84 (2)      |               |

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