



# Crystal structure of $\text{Sc}_{1.91}\text{In}_{1.39}\text{Mo}_{15}\text{Se}_{19}$ , containing $\text{Mo}_6$ and $\text{Mo}_9$ clusters

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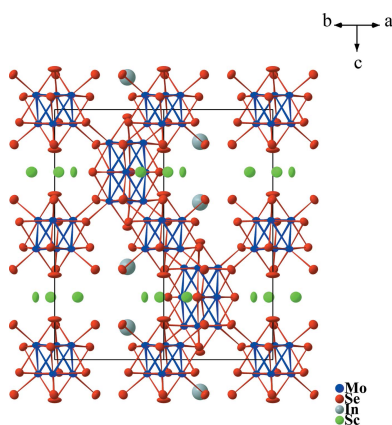
The structure of scandium indium pentadecamolybdenum nonadecaselenide,  $\text{Sc}_{1.91}\text{In}_{1.39}\text{Mo}_{15}\text{Se}_{19}$ , is isotypic with  $\text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19}$  [Grüttner *et al.* (1979), *Acta Cryst. B* **35**, 285–292]. It is characterized by two cluster units  $\text{Mo}_6\text{Se}_8^i\text{Se}_6^a$  and  $\text{Mo}_9\text{Se}_{11}^i\text{Se}_6^a$  (where *i* represents inner and *a* apical atoms) that are present in a 1:1 ratio. The cluster units are centered at Wyckoff positions  $2b$  and  $2c$  and have point-group symmetry  $\bar{3}$  and  $\bar{6}$ , respectively. The clusters are interconnected through additional Mo–Se bonds. Sc–Se and In–Se bonds complete the structural set-up. In the title compound, the  $\text{Sc}^{3+}$  cations replace the trivalent indium atoms present in  $\text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19}$ , and a deficiency is observed at the monovalent indium site. One Mo, one Se and the Sc atom are situated on mirror planes, whereas two other Se atoms and the In atom are situated on threefold rotation axes.

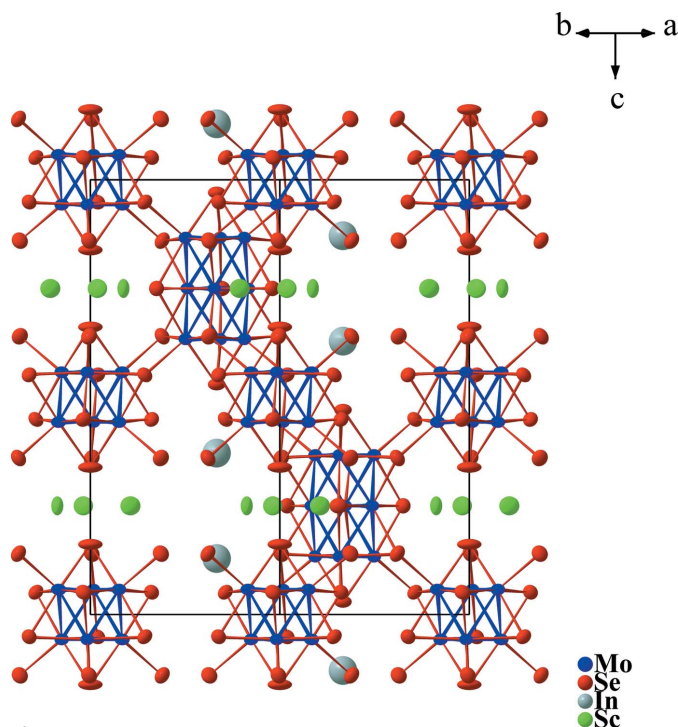
## 1. Chemical context

From a crystal–chemical point of view, reduced molybdenum selenides  $\text{In}_3\text{Mo}_{15}\text{Se}_{19}$  (Grüttner *et al.*, 1979) constitute an interesting family of compounds. Indeed, their crystal structures contain an equal mixture of  $\text{Mo}_6$  and  $\text{Mo}_9$  cluster units with the In atoms occupying two crystallographically different positions depending on their formal oxidation state of +1 or +3. 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). Recently, we have shown that the  $\text{In}^{3+}$  cation can be replaced by other trivalent cations such as  $\text{Ho}^{3+}$  (resulting in a compound with composition  $\text{Ho}_{0.76}\text{In}_{1.68}\text{Mo}_{15}\text{Se}_{19}$ ; Salloum *et al.*, 2006) or  $\text{V}^{3+}$  ( $\text{V}_{1.42}\text{In}_{1.83}\text{Mo}_{15}\text{Se}_{19}$ ; Gougeon *et al.*, 2010), and the  $\text{In}^+$  cation by  $\text{K}^+$  ( $\text{In}_{0.87}\text{K}_2\text{Mo}_{15}\text{Se}_{19}$ ; Salloum *et al.*, 2007). We present here the crystal structure of  $\text{Sc}_{1.91}\text{In}_{1.39}\text{Mo}_{15}\text{Se}_{19}$  in which scandium atoms replace the trivalent indium atoms.

## 2. Structural commentary

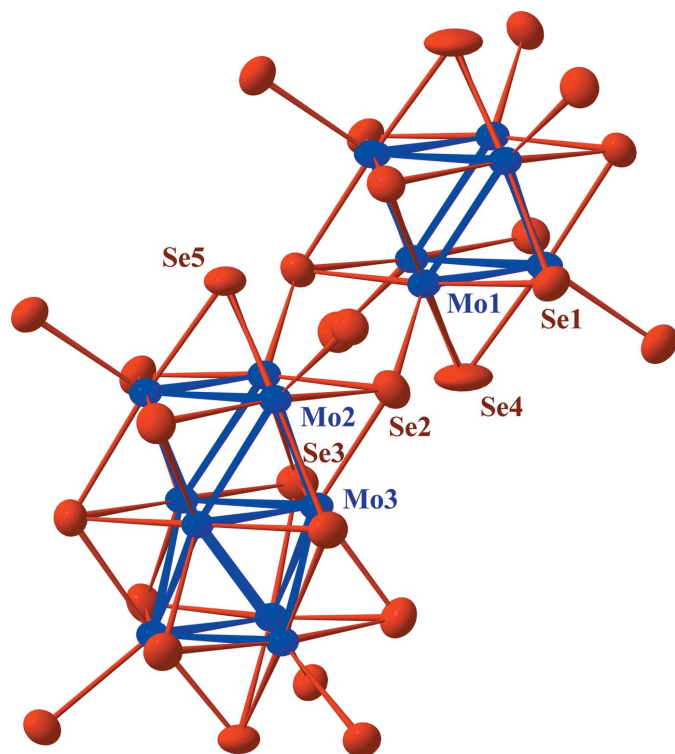
The Mo–Se framework of the title compound consists of the cluster units  $\text{Mo}_6\text{Se}_8^i\text{Se}_6^a$  and  $\text{Mo}_9\text{Se}_{11}^i\text{Se}_6^a$  in a 1:1 ratio (for details of the *i*- and *a*-type ligand notation, see: Schäfer & von Schnering, 1964). Both cluster units are interconnected through additional Mo–Se bonds (Table 1, Figs. 1 and 2). The first unit can be described as an  $\text{Mo}_6$  octahedron surrounded by eight face-capping inner  $\text{Se}^i$  and six apical  $\text{Se}^a$  ligands. The  $\text{Mo}_9$  cluster is surrounded by 11  $\text{Se}^i$  atoms capping one or two faces of the bioctahedron and six  $\text{Se}^a$  ligands above the apical Mo atoms. The  $\text{Mo}_6\text{Se}_8^i\text{Se}_6^a$  and  $\text{Mo}_9\text{Se}_{11}^i\text{Se}_6^a$  units are centered at Wyckoff positions  $2b$  and  $2c$  and have point-group





**Figure 1**  
View of the crystal structure of  $\text{Sc}_{1.91}\text{In}_{1.39}\text{Mo}_{15}\text{Se}_{19}$  along  $[110]$ . Displacement ellipsoids are drawn at the 97% probability level.

symmetry  $\bar{3}$  and  $\bar{6}$ , respectively. The Mo—Mo distances within the  $\text{Mo}_6$  cluster are 2.6995 (6) Å for the distances of the Mo



**Figure 2**  
Plot showing the atom-numbering scheme and the interunit linkage of the  $\text{Mo}_9\text{Se}_{11}\text{Se}_6$  and  $\text{Mo}_6\text{Se}_8\text{Se}_6$  cluster units. Displacement ellipsoids are drawn at the 97% probability level.

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

Mo1—Se4	2.5480 (6)	Mo3—Se2	2.5780 (5)
Mo1—Se1 <sup>i</sup>	2.5488 (5)	Mo3—Se3 <sup>iii</sup>	2.5884 (7)
Mo1—Se1	2.5749 (5)	Mo3—Se3	2.5900 (7)
Mo1—Se1 <sup>ii</sup>	2.6145 (5)	Mo3—Mo3 <sup>iii</sup>	2.7127 (8)
Mo1—Se2	2.6531 (5)	In—Se5	3.0662 (13)
Mo1—Mo1 <sup>ii</sup>	2.6995 (6)	In—Se2 <sup>vii</sup>	3.1273 (4)
Mo1—Mo1 <sup>i</sup>	2.7179 (5)	In—Se2 <sup>viii</sup>	3.1273 (4)
Mo2—Se5	2.5290 (6)	In—Se2 <sup>i</sup>	3.1273 (4)
Mo2—Se2	2.5931 (5)	In—Se1 <sup>vii</sup>	3.4912 (6)
Mo2—Se2 <sup>iii</sup>	2.6275 (5)	In—Se1 <sup>i</sup>	3.4912 (6)
Mo2—Mo2 <sup>iv</sup>	2.6460 (6)	In—Se1 <sup>viii</sup>	3.4912 (6)
Mo2—Se1 <sup>v</sup>	2.6581 (5)	Sc—Se4 <sup>vi</sup>	2.5691 (15)
Mo2—Se3 <sup>iii</sup>	2.6965 (4)	Sc—Se3 <sup>ii</sup>	2.696 (2)
Mo2—Mo3 <sup>iii</sup>	2.7196 (4)	Sc—Se2 <sup>ix</sup>	2.8056 (12)
Mo2—Mo3	2.7675 (4)	Sc—Se2 <sup>x</sup>	2.8056 (12)
Mo3—Se2 <sup>vi</sup>	2.5780 (5)	Sc—Se3 <sup>ix</sup>	2.931 (2)

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

triangles formed by the Mo1 atoms related through the threefold axis, and 2.7179 (5) Å for the distances between these triangles. The Mo—Mo distances within the  $\text{Mo}_9$  clusters are 2.6460 (6) and 2.7127 (8) Å in the triangles formed by the atoms Mo2 and Mo3, respectively, and 2.7196 (4) and 2.7675 (4) Å for those between the  $\text{Mo}_2$  and  $\text{Mo}_3$  triangles. The Se atoms bridge either one (Se1, Se2, Se4 and Se5) or two (Se3) triangular faces of the Mo clusters. Moreover, atoms Se1 and Se2 are linked to an Mo atom of a neighboring cluster. The Mo—Se bond lengths range from 2.5480 (6) to 2.6531 (5) Å within the  $\text{Mo}_6\text{Se}_8\text{Se}_6^i$  unit, and from 2.5290 (6) to 2.6966 (4) Å within the  $\text{Mo}_9\text{Se}_{11}\text{Se}_6^a$  unit. Each  $\text{Mo}_9\text{Se}_{11}\text{Se}_6^a$  cluster is interconnected by six  $\text{Mo}_6\text{Se}_8\text{Se}_6^a$  units (and *vice versa*) via Mo2—Se1 bonds (and Mo1—Se2 bonds, respectively), forming the three-dimensional Mo—Se framework, the connectivity formula of which is  $\text{Mo}_9\text{Se}_5\text{Se}_{6/2}^{i-a}\text{Se}_{6/2}^{a-i}$ ,  $\text{Mo}_6\text{Se}_2\text{Se}_{6/2}^{i-a}\text{Se}_{6/2}^{a-i}$ . It results from this arrangement that the shortest intercluster Mo1—Mo2 distance is 3.4361 (5) Å, indicating only weak metal··metal interactions.

Comparison of the Mo—Mo and Mo—Se distances with those of the other substituted compounds  $\text{Ho}_{0.76}\text{In}_{1.68}\text{Mo}_{15}\text{Se}_{19}$ ,  $\text{In}_{0.87}\text{K}_2\text{Mo}_{15}\text{Se}_{19}$  and  $\text{V}_{1.42}\text{In}_{1.83}\text{Mo}_{15}\text{Se}_{19}$  does not reveal great differences although the cationic charges are different in the four compounds. The In<sup>+</sup> cations are surrounded by seven Se atoms, forming a distorted tricapped tetrahedron as in  $\text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19}$ . The Se5 and Se2 atoms forming the tetrahedron are at 3.0662 (13) and 3.1273 (4) Å from the In<sup>+</sup> cation, and the capping Se1 atoms are at 3.4912 (6) Å. While in  $\text{In}_{2.9}\text{Mo}_{15}\text{Se}_{19}$  the monovalent In site is fully occupied, in the title compound it is only has 69.5 (3)% occupancy. This deficiency probably results from the higher temperature used during the crystal-growth process, which led to a loss of indium and selenium because of the high volatility of these elements at 1773 K. The Sc<sup>3+</sup> cations, as the In<sup>3+</sup> cations in the  $\text{In}_3\text{Mo}_{15}\text{Se}_{19}$  compounds, occupy partially at 63.8 (6)% a triangular group of distorted octahedral cavities, which are formed by two  $\text{Mo}_6\text{Se}_8\text{Se}_6^a$  and three  $\text{Mo}_9\text{Se}_{11}\text{Se}_6^a$

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	Sc <sub>1.91</sub> In <sub>1.39</sub> Mo <sub>15</sub> Se <sub>19</sub>
$M_r$	3185.04
Crystal system, space group	Hexagonal, $P6_3/m$
Temperature (K)	293
$a, c$ (Å)	9.7530 (2), 19.3977 (2)
$V$ (Å <sup>3</sup> )	1597.93 (7)
$Z$	2
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	28.65
Crystal size (mm)	0.06 × 0.05 × 0.04
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	Analytical (de Meulenaar & Tompa, 1965)
$T_{\min}, T_{\max}$	0.279, 0.424
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	31413, 2414, 1847
$R_{\text{int}}$	0.073
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.807
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.063, 1.08
No. of reflections	2414
No. of parameters	67
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	2.22, -1.97

Computer programs: COLLECT (Nonius, 1998), EVALCCD (Duisenberg *et al.*, 2003), SIR97 (Altomare *et al.*, 1999), SHELXL2014/6 (Sheldrick, 2015) and DIAMOND (Bergerhoff, 1996).

units, around the threefold rotation axis. The Sc–Se distances are in the 2.5691 (15)–2.931 (2) Å range.

### 3. Synthesis and crystallization

Single crystals of Sc<sub>1.91</sub>In<sub>1.39</sub>Mo<sub>15</sub>Se<sub>19</sub> were obtained from a mixture of Sc<sub>2</sub>Se<sub>3</sub>, MoSe<sub>2</sub>, InSe and Mo with a nominal composition Sc<sub>2</sub>In<sub>2</sub>Mo<sub>15</sub>Se<sub>19</sub>. Before use, Mo powder was reduced under H<sub>2</sub> flowing gas at 1273 K for ten h in order to eliminate any trace of oxygen. The binaries Sc<sub>2</sub>Se<sub>3</sub>, MoSe<sub>2</sub>, InSe were obtained by heating stoichiometric mixtures of the elements in sealed evacuated silica tubes for about two days. All handling of materials was performed 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<sup>-1</sup> up to 1773 K, the temperature which was held for 48 h, then cooled at 100 K h<sup>-1</sup> down to 1373 K and finally furnace cooled.

### 4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The highest and lowest remaining electron densities are located 0.66 and 0.62 Å from the In site, respectively. Refinement of the occupancy factors of the Sc and In atoms led to the final composition Sc<sub>1.914</sub>(12)In<sub>1.390</sub>(6)Mo<sub>15</sub>Se<sub>19</sub>.

### Acknowledgements

Intensity data were collected on the Nonius KappaCCD X-ray diffractometer system of the Centre de diffractométrie de l'Université de Rennes I (URL: [www.cdifx.univ-rennes1.fr](http://www.cdifx.univ-rennes1.fr)).

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## supporting information

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### Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *COLLECT* (Nonius, 1998); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014/6* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *SHELXL2014/6* (Sheldrick, 2015).

### Scandium indium pentadecamolybdenum nonadecaselenide

#### Crystal data

$\text{Sc}_{1.91}\text{In}_{1.39}\text{Mo}_{15}\text{Se}_{19}$   
 $M_r = 3185.04$   
 Hexagonal,  $P6_3/m$   
 $a = 9.7530$  (2) Å  
 $c = 19.3977$  (2) Å  
 $V = 1597.93$  (7) Å<sup>3</sup>  
 $Z = 2$

$F(000) = 2769$   
 $D_x = 6.620$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71069$  Å  
 $\mu = 28.65$  mm<sup>-1</sup>  
 $T = 293$  K  
 Irregular block, black  
 $0.06 \times 0.05 \times 0.04$  mm

#### Data collection

Nonius KappaCCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  scans ( $\kappa = 0$ ) + additional  $\omega$  scans  
 Absorption correction: analytical  
 (de Meulenaar & Tompa, 1965)  
 $T_{\min} = 0.279$ ,  $T_{\max} = 0.424$

31413 measured reflections  
 2414 independent reflections  
 1847 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.073$   
 $\theta_{\max} = 35.0^\circ$ ,  $\theta_{\min} = 2.4^\circ$   
 $h = -13 \rightarrow 15$   
 $k = -15 \rightarrow 13$   
 $l = -31 \rightarrow 26$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.063$   
 $S = 1.08$   
 2414 reflections  
 67 parameters  
 0 restraints

$w = 1/[\sigma^2(F_o^2) + (0.0228P)^2 + 7.5263P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 2.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.96$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL*,  
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.00065 (4)

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mo1	0.16732 (4)	0.01628 (4)	0.55740 (2)	0.00813 (7)	
Mo2	0.68442 (4)	0.18633 (4)	0.63321 (2)	0.00769 (7)	
Mo3	0.51261 (5)	0.16694 (5)	0.7500	0.00748 (8)	
Se1	0.03573 (5)	−0.28735 (5)	0.55124 (2)	0.01007 (8)	
Se2	0.37937 (5)	0.00705 (5)	0.64001 (2)	0.01114 (9)	
Se3	0.34923 (7)	0.30997 (7)	0.7500	0.01107 (11)	
Se4	0.0000	0.0000	0.66131 (3)	0.01933 (16)	
Se5	0.6667	0.3333	0.52931 (3)	0.01116 (13)	
In	0.6667	0.3333	0.37124 (6)	0.0358 (4)	0.695 (3)
Sc	−0.2115 (2)	−0.1745 (2)	0.7500	0.0143 (5)	0.638 (6)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mo1	0.01005 (15)	0.00828 (15)	0.00598 (13)	0.00453 (12)	0.00026 (9)	0.00006 (9)
Mo2	0.00846 (14)	0.00829 (14)	0.00626 (12)	0.00415 (12)	−0.00015 (9)	−0.00030 (9)
Mo3	0.0087 (2)	0.0085 (2)	0.00563 (16)	0.00458 (16)	0.000	0.000
Se1	0.01139 (18)	0.00980 (18)	0.00960 (15)	0.00572 (15)	0.00112 (12)	0.00197 (12)
Se2	0.00992 (18)	0.01101 (19)	0.01187 (16)	0.00477 (14)	−0.00272 (12)	−0.00153 (12)
Se3	0.0098 (3)	0.0142 (3)	0.0104 (2)	0.0069 (2)	0.000	0.000
Se4	0.0264 (3)	0.0264 (3)	0.0053 (3)	0.01318 (13)	0.000	0.000
Se5	0.0136 (2)	0.0136 (2)	0.0063 (2)	0.00679 (10)	0.000	0.000
In	0.0355 (5)	0.0355 (5)	0.0363 (6)	0.0178 (2)	0.000	0.000
Sc	0.0176 (10)	0.0064 (8)	0.0159 (8)	0.0038 (7)	0.000	0.000

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

Mo1—Se4	2.5480 (6)	Se3—Sc <sup>ii</sup>	2.931 (2)
Mo1—Se1 <sup>i</sup>	2.5488 (5)	Se4—Mo1 <sup>iii</sup>	2.5479 (6)
Mo1—Se1	2.5749 (5)	Se4—Mo1 <sup>ii</sup>	2.5479 (6)
Mo1—Se1 <sup>ii</sup>	2.6145 (5)	Se4—Sc <sup>iii</sup>	2.5691 (15)
Mo1—Se2	2.6531 (5)	Se4—Sc <sup>ii</sup>	2.5691 (15)
Mo1—Mo1 <sup>ii</sup>	2.6995 (6)	Se4—Sc	2.5691 (15)
Mo1—Mo1 <sup>iii</sup>	2.6995 (6)	Se5—Mo2 <sup>v</sup>	2.5290 (6)
Mo1—Mo1 <sup>i</sup>	2.7179 (5)	Se5—Mo2 <sup>vi</sup>	2.5290 (6)
Mo1—Mo1 <sup>iv</sup>	2.7179 (5)	In—Se5	3.0662 (13)
Mo2—Se5	2.5290 (6)	In—Se2 <sup>xi</sup>	3.1273 (4)
Mo2—Se2	2.5931 (5)	In—Se2 <sup>xii</sup>	3.1273 (4)
Mo2—Se2 <sup>v</sup>	2.6275 (5)	In—Se2 <sup>i</sup>	3.1273 (4)

Mo2—Mo2 <sup>vi</sup>	2.6460 (6)	In—Se1 <sup>xi</sup>	3.4912 (6)
Mo2—Mo2 <sup>v</sup>	2.6460 (6)	In—Se1 <sup>i</sup>	3.4912 (6)
Mo2—Se1 <sup>vii</sup>	2.6581 (5)	In—Se1 <sup>xii</sup>	3.4912 (6)
Mo2—Se3 <sup>v</sup>	2.6965 (4)	In—Se3 <sup>iv</sup>	4.2657 (8)
Mo2—Mo3 <sup>v</sup>	2.7196 (4)	In—Se3 <sup>xiii</sup>	4.2657 (8)
Mo2—Mo3	2.7675 (4)	In—Se3 <sup>xiv</sup>	4.2657 (8)
Mo3—Se2 <sup>viii</sup>	2.5780 (5)	In—Sc <sup>xv</sup>	4.5565 (18)
Mo3—Se2	2.5780 (5)	In—Sc <sup>xvi</sup>	4.5565 (18)
Mo3—Se3 <sup>v</sup>	2.5884 (7)	In—Sc <sup>xvii</sup>	4.5565 (18)
Mo3—Se3	2.5900 (7)	Sc—Se4 <sup>viii</sup>	2.5691 (15)
Mo3—Mo3 <sup>v</sup>	2.7127 (8)	Sc—Se3 <sup>ii</sup>	2.696 (2)
Mo3—Mo3 <sup>vi</sup>	2.7127 (8)	Sc—Se2 <sup>iii</sup>	2.8056 (12)
Mo3—Mo2 <sup>ix</sup>	2.7196 (4)	Sc—Se2 <sup>xviii</sup>	2.8056 (12)
Mo3—Mo2 <sup>vi</sup>	2.7196 (4)	Sc—Mo3 <sup>iii</sup>	2.8760 (18)
Mo3—Mo2 <sup>viii</sup>	2.7675 (4)	Sc—Se3 <sup>iii</sup>	2.931 (2)
Mo3—Sc <sup>ii</sup>	2.8760 (18)	Sc—Sc <sup>iii</sup>	3.305 (3)
Se1—Mo1 <sup>iv</sup>	2.5488 (5)	Sc—Sc <sup>ii</sup>	3.305 (3)
Se1—Mo1 <sup>iii</sup>	2.6145 (5)	Sc—Mo1 <sup>xviii</sup>	3.7775 (4)
Se1—Mo2 <sup>x</sup>	2.6581 (5)	Sc—Mo1 <sup>iii</sup>	3.7775 (4)
Se2—Mo2 <sup>vi</sup>	2.6275 (5)	Sc—Mo2 <sup>x</sup>	4.0216 (15)
Se2—Sc <sup>ii</sup>	2.8056 (12)	Sc—Mo2 <sup>xix</sup>	4.0216 (15)
Se3—Mo3 <sup>vi</sup>	2.5884 (7)	Sc—Se1 <sup>xviii</sup>	4.3993 (10)
Se3—Mo2 <sup>ix</sup>	2.6966 (4)	Sc—Se1 <sup>iii</sup>	4.3993 (10)
Se3—Mo2 <sup>vi</sup>	2.6966 (4)	Sc—In <sup>xvi</sup>	4.5564 (18)
Se3—Sc <sup>iii</sup>	2.696 (2)		
Se4—Mo1—Se1 <sup>i</sup>	176.406 (19)	Mo2 <sup>ix</sup> —Mo3—Mo2	145.97 (2)
Se4—Mo1—Se1	91.698 (13)	Mo2 <sup>vi</sup> —Mo3—Mo2	57.653 (13)
Se1 <sup>i</sup> —Mo1—Se1	89.030 (13)	Se2 <sup>viii</sup> —Mo3—Mo2 <sup>viii</sup>	57.907 (12)
Se4—Mo1—Se1 <sup>ii</sup>	90.788 (13)	Se2—Mo3—Mo2 <sup>viii</sup>	145.46 (2)
Se1 <sup>i</sup> —Mo1—Se1 <sup>ii</sup>	88.161 (13)	Se3 <sup>v</sup> —Mo3—Mo2 <sup>viii</sup>	60.349 (12)
Se1—Mo1—Se1 <sup>ii</sup>	174.05 (2)	Se3—Mo3—Mo2 <sup>viii</sup>	118.538 (13)
Se4—Mo1—Se2	90.338 (16)	Mo3 <sup>v</sup> —Mo3—Mo2 <sup>viii</sup>	59.495 (13)
Se1 <sup>i</sup> —Mo1—Se2	93.220 (16)	Mo3 <sup>vi</sup> —Mo3—Mo2 <sup>viii</sup>	88.794 (12)
Se1—Mo1—Se2	86.430 (16)	Mo2 <sup>ix</sup> —Mo3—Mo2 <sup>viii</sup>	57.654 (13)
Se1 <sup>ii</sup> —Mo1—Se2	98.964 (16)	Mo2 <sup>vi</sup> —Mo3—Mo2 <sup>viii</sup>	145.97 (2)
Se4—Mo1—Mo1 <sup>ii</sup>	58.012 (9)	Mo2—Mo3—Mo2 <sup>viii</sup>	109.89 (2)
Se1 <sup>i</sup> —Mo1—Mo1 <sup>ii</sup>	118.654 (14)	Se2 <sup>viii</sup> —Mo3—Sc <sup>ii</sup>	61.629 (19)
Se1—Mo1—Mo1 <sup>ii</sup>	119.304 (17)	Se2—Mo3—Sc <sup>ii</sup>	61.629 (19)
Se1 <sup>ii</sup> —Mo1—Mo1 <sup>ii</sup>	57.940 (16)	Se3 <sup>v</sup> —Mo3—Sc <sup>ii</sup>	118.59 (5)
Se2—Mo1—Mo1 <sup>ii</sup>	137.271 (14)	Se3—Mo3—Sc <sup>ii</sup>	64.60 (4)
Se4—Mo1—Mo1 <sup>iii</sup>	58.012 (9)	Mo3 <sup>v</sup> —Mo3—Sc <sup>ii</sup>	177.02 (5)
Se1 <sup>i</sup> —Mo1—Mo1 <sup>iii</sup>	119.634 (13)	Mo3 <sup>vi</sup> —Mo3—Sc <sup>ii</sup>	122.98 (5)
Se1—Mo1—Mo1 <sup>iii</sup>	59.376 (17)	Mo2 <sup>ix</sup> —Mo3—Sc <sup>ii</sup>	91.85 (3)
Se1 <sup>ii</sup> —Mo1—Mo1 <sup>iii</sup>	117.870 (16)	Mo2 <sup>vi</sup> —Mo3—Sc <sup>ii</sup>	91.85 (3)
Se2—Mo1—Mo1 <sup>iii</sup>	129.426 (16)	Mo2—Mo3—Sc <sup>ii</sup>	119.536 (18)
Mo1 <sup>ii</sup> —Mo1—Mo1 <sup>iii</sup>	60.0	Mo2 <sup>viii</sup> —Mo3—Sc <sup>ii</sup>	119.536 (18)
Se4—Mo1—Mo1 <sup>i</sup>	118.212 (12)	Mo1 <sup>iv</sup> —Se1—Mo1	64.071 (16)

Se1 <sup>i</sup> —Mo1—Mo1 <sup>i</sup>	58.430 (15)	Mo1 <sup>iv</sup> —Se1—Mo1 <sup>iii</sup>	63.509 (16)
Se1—Mo1—Mo1 <sup>i</sup>	117.048 (15)	Mo1—Se1—Mo1 <sup>iii</sup>	62.685 (17)
Se1 <sup>ii</sup> —Mo1—Mo1 <sup>i</sup>	57.068 (11)	Mo1 <sup>iv</sup> —Se1—Mo2 <sup>x</sup>	131.401 (19)
Se2—Mo1—Mo1 <sup>i</sup>	140.439 (16)	Mo1—Se1—Mo2 <sup>x</sup>	128.246 (18)
Mo1 <sup>ii</sup> —Mo1—Mo1 <sup>i</sup>	60.224 (8)	Mo1 <sup>iii</sup> —Se1—Mo2 <sup>x</sup>	81.335 (15)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>i</sup>	90.0	Mo3—Se2—Mo2	64.712 (15)
Se4—Mo1—Mo1 <sup>iv</sup>	118.212 (12)	Mo3—Se2—Mo2 <sup>vi</sup>	62.984 (14)
Se1 <sup>i</sup> —Mo1—Mo1 <sup>iv</sup>	59.423 (15)	Mo2—Se2—Mo2 <sup>vi</sup>	60.903 (17)
Se1—Mo1—Mo1 <sup>iv</sup>	57.499 (11)	Mo3—Se2—Mo1	130.17 (2)
Se1 <sup>ii</sup> —Mo1—Mo1 <sup>iv</sup>	116.606 (15)	Mo2—Se2—Mo1	126.687 (18)
Se2—Mo1—Mo1 <sup>iv</sup>	132.232 (15)	Mo2 <sup>vi</sup> —Se2—Mo1	81.187 (15)
Mo1 <sup>ii</sup> —Mo1—Mo1 <sup>iv</sup>	90.0	Mo3—Se2—Sc <sup>ii</sup>	64.42 (3)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>iv</sup>	60.224 (8)	Mo2—Se2—Sc <sup>ii</sup>	129.13 (3)
Mo1 <sup>i</sup> —Mo1—Mo1 <sup>iv</sup>	59.550 (15)	Mo2 <sup>vi</sup> —Se2—Sc <sup>ii</sup>	95.44 (4)
Se5—Mo2—Se2	92.412 (13)	Mo1—Se2—Sc <sup>ii</sup>	87.53 (3)
Se5—Mo2—Se2 <sup>v</sup>	91.604 (13)	Mo3 <sup>vi</sup> —Se3—Mo3	63.18 (2)
Se2—Mo2—Se2 <sup>v</sup>	174.13 (2)	Mo3 <sup>vi</sup> —Se3—Mo2 <sup>ix</sup>	63.118 (13)
Se5—Mo2—Mo2 <sup>vi</sup>	58.457 (9)	Mo3—Se3—Mo2 <sup>ix</sup>	61.881 (13)
Se2—Mo2—Mo2 <sup>vi</sup>	60.191 (17)	Mo3 <sup>vi</sup> —Se3—Mo2 <sup>vi</sup>	63.118 (13)
Se2 <sup>v</sup> —Mo2—Mo2 <sup>vi</sup>	118.823 (16)	Mo3—Se3—Mo2 <sup>vi</sup>	61.881 (14)
Se5—Mo2—Mo2 <sup>v</sup>	58.457 (9)	Mo2 <sup>ix</sup> —Se3—Mo2 <sup>vi</sup>	114.31 (2)
Se2—Mo2—Mo2 <sup>v</sup>	120.106 (17)	Mo3 <sup>vi</sup> —Se3—Sc <sup>iii</sup>	162.59 (5)
Se2 <sup>v</sup> —Mo2—Mo2 <sup>v</sup>	58.906 (16)	Mo3—Se3—Sc <sup>iii</sup>	134.23 (5)
Mo2 <sup>vi</sup> —Mo2—Mo2 <sup>v</sup>	60.0	Mo2 <sup>ix</sup> —Se3—Sc <sup>iii</sup>	121.404 (15)
Se5—Mo2—Se1 <sup>vii</sup>	90.196 (15)	Mo2 <sup>vi</sup> —Se3—Sc <sup>iii</sup>	121.404 (15)
Se2—Mo2—Se1 <sup>vii</sup>	85.764 (16)	Mo3 <sup>vi</sup> —Se3—Sc <sup>ii</sup>	125.62 (4)
Se2 <sup>v</sup> —Mo2—Se1 <sup>vii</sup>	98.510 (16)	Mo3—Se3—Sc <sup>ii</sup>	62.43 (4)
Mo2 <sup>vi</sup> —Mo2—Se1 <sup>vii</sup>	129.579 (16)	Mo2 <sup>ix</sup> —Se3—Sc <sup>ii</sup>	91.14 (2)
Mo2 <sup>v</sup> —Mo2—Se1 <sup>vii</sup>	137.688 (14)	Mo2 <sup>vi</sup> —Se3—Sc <sup>ii</sup>	91.14 (2)
Se5—Mo2—Se3 <sup>v</sup>	175.172 (19)	Sc <sup>iii</sup> —Se3—Sc <sup>ii</sup>	71.79 (8)
Se2—Mo2—Se3 <sup>v</sup>	85.424 (18)	Mo1 <sup>iii</sup> —Se4—Mo1 <sup>ii</sup>	63.974 (19)
Se2 <sup>v</sup> —Mo2—Se3 <sup>v</sup>	90.244 (18)	Mo1 <sup>iii</sup> —Se4—Mo1	63.975 (19)
Mo2 <sup>vi</sup> —Mo2—Se3 <sup>v</sup>	116.797 (15)	Mo1 <sup>ii</sup> —Se4—Mo1	63.974 (19)
Mo2 <sup>v</sup> —Mo2—Se3 <sup>v</sup>	119.114 (14)	Mo1 <sup>iii</sup> —Se4—Sc <sup>iii</sup>	148.00 (4)
Se1 <sup>viii</sup> —Mo2—Se3 <sup>v</sup>	93.942 (17)	Mo1 <sup>ii</sup> —Se4—Sc <sup>iii</sup>	95.16 (3)
Se5—Mo2—Mo3 <sup>v</sup>	120.527 (17)	Mo1—Se4—Sc <sup>iii</sup>	130.64 (4)
Se2—Mo2—Mo3 <sup>v</sup>	116.554 (16)	Mo1 <sup>iii</sup> —Se4—Sc <sup>ii</sup>	130.64 (4)
Se2 <sup>v</sup> —Mo2—Mo3 <sup>v</sup>	57.619 (13)	Mo1 <sup>ii</sup> —Se4—Sc <sup>ii</sup>	148.00 (4)
Mo2 <sup>vi</sup> —Mo2—Mo3 <sup>v</sup>	91.213 (12)	Mo1—Se4—Sc <sup>ii</sup>	95.16 (3)
Mo2 <sup>v</sup> —Mo2—Mo3 <sup>v</sup>	62.083 (12)	Sc <sup>iii</sup> —Se4—Sc <sup>ii</sup>	80.06 (5)
Se1 <sup>viii</sup> —Mo2—Mo3 <sup>v</sup>	138.895 (18)	Mo1 <sup>iii</sup> —Se4—Sc	95.16 (3)
Se3 <sup>v</sup> —Mo2—Mo3 <sup>v</sup>	57.133 (16)	Mo1 <sup>ii</sup> —Se4—Sc	130.64 (4)
Se5—Mo2—Mo3	118.709 (16)	Mo1—Se4—Sc	148.00 (4)
Se2—Mo2—Mo3	57.381 (13)	Sc <sup>iii</sup> —Se4—Sc	80.06 (5)
Se2 <sup>v</sup> —Mo2—Mo3	116.832 (16)	Sc <sup>ii</sup> —Se4—Sc	80.06 (5)
Mo2 <sup>vi</sup> —Mo2—Mo3	60.264 (12)	Mo2 <sup>v</sup> —Se5—Mo2	63.086 (18)
Mo2 <sup>v</sup> —Mo2—Mo3	90.162 (12)	Mo2 <sup>v</sup> —Se5—Mo2 <sup>vi</sup>	63.086 (18)
Se1 <sup>viii</sup> —Mo2—Mo3	131.676 (18)	Mo2—Se5—Mo2 <sup>vi</sup>	63.086 (18)

Se3 <sup>v</sup> —Mo2—Mo3	56.533 (15)	Se4 <sup>viii</sup> —Sc—Se4	84.08 (6)
Mo3 <sup>v</sup> —Mo2—Mo3	59.250 (17)	Se4 <sup>viii</sup> —Sc—Se3 <sup>ii</sup>	88.06 (5)
Se2 <sup>viii</sup> —Mo3—Se2	111.71 (3)	Se4—Sc—Se3 <sup>ii</sup>	88.06 (5)
Se2 <sup>viii</sup> —Mo3—Se3 <sup>v</sup>	87.997 (16)	Se4 <sup>viii</sup> —Sc—Se2 <sup>iii</sup>	163.50 (8)
Se2—Mo3—Se3 <sup>v</sup>	87.997 (16)	Se4—Sc—Se2 <sup>iii</sup>	86.578 (17)
Se2 <sup>viii</sup> —Mo3—Se3	93.784 (17)	Se3 <sup>ii</sup> —Sc—Se2 <sup>iii</sup>	105.20 (5)
Se2—Mo3—Se3	93.784 (17)	Se4 <sup>viii</sup> —Sc—Se2 <sup>xviii</sup>	86.579 (17)
Se3 <sup>v</sup> —Mo3—Se3	176.82 (2)	Se4—Sc—Se2 <sup>xviii</sup>	163.51 (8)
Se2 <sup>viii</sup> —Mo3—Mo3 <sup>v</sup>	117.324 (17)	Se3 <sup>ii</sup> —Sc—Se2 <sup>xviii</sup>	105.20 (5)
Se2—Mo3—Mo3 <sup>v</sup>	117.324 (17)	Se2 <sup>iii</sup> —Sc—Se2 <sup>xviii</sup>	99.02 (6)
Se3 <sup>v</sup> —Mo3—Mo3 <sup>v</sup>	58.44 (2)	Se4 <sup>viii</sup> —Sc—Mo3 <sup>iii</sup>	120.92 (5)
Se3—Mo3—Mo3 <sup>v</sup>	118.38 (2)	Se4—Sc—Mo3 <sup>iii</sup>	120.92 (5)
Se2 <sup>viii</sup> —Mo3—Mo3 <sup>vi</sup>	120.613 (15)	Se3 <sup>ii</sup> —Sc—Mo3 <sup>iii</sup>	138.83 (8)
Se2—Mo3—Mo3 <sup>vi</sup>	120.614 (15)	Se2 <sup>iii</sup> —Sc—Mo3 <sup>iii</sup>	53.95 (3)
Se3 <sup>v</sup> —Mo3—Mo3 <sup>vi</sup>	118.44 (2)	Se2 <sup>xviii</sup> —Sc—Mo3 <sup>iii</sup>	53.95 (3)
Se3—Mo3—Mo3 <sup>vi</sup>	58.38 (2)	Se4 <sup>viii</sup> —Sc—Se3 <sup>iii</sup>	83.19 (5)
Mo3 <sup>v</sup> —Mo3—Mo3 <sup>vi</sup>	60.0	Se4—Sc—Se3 <sup>iii</sup>	83.19 (5)
Se2 <sup>viii</sup> —Mo3—Mo2 <sup>ix</sup>	59.397 (12)	Se3 <sup>ii</sup> —Sc—Se3 <sup>iii</sup>	168.21 (8)
Se2—Mo3—Mo2 <sup>ix</sup>	150.43 (2)	Se2 <sup>iii</sup> —Sc—Se3 <sup>iii</sup>	82.23 (4)
Se3 <sup>v</sup> —Mo3—Mo2 <sup>ix</sup>	118.002 (13)	Se2 <sup>xviii</sup> —Sc—Se3 <sup>iii</sup>	82.23 (4)
Se3—Mo3—Mo2 <sup>ix</sup>	60.986 (12)	Mo3 <sup>iii</sup> —Sc—Se3 <sup>iii</sup>	52.97 (3)
Mo3 <sup>v</sup> —Mo3—Mo2 <sup>ix</sup>	89.795 (12)	Se4 <sup>viii</sup> —Sc—Sc <sup>iii</sup>	49.97 (2)
Mo3 <sup>vi</sup> —Mo3—Mo2 <sup>ix</sup>	61.256 (13)	Se4—Sc—Sc <sup>iii</sup>	49.97 (2)
Se2 <sup>viii</sup> —Mo3—Mo2 <sup>vi</sup>	150.43 (2)	Se3 <sup>ii</sup> —Sc—Sc <sup>iii</sup>	57.39 (6)
Se2—Mo3—Mo2 <sup>vi</sup>	59.397 (12)	Se2 <sup>iii</sup> —Sc—Sc <sup>iii</sup>	129.92 (3)
Se3 <sup>v</sup> —Mo3—Mo2 <sup>vi</sup>	118.002 (13)	Se2 <sup>xviii</sup> —Sc—Sc <sup>iii</sup>	129.92 (3)
Se3—Mo3—Mo2 <sup>vi</sup>	60.986 (12)	Mo3 <sup>iii</sup> —Sc—Sc <sup>iii</sup>	163.78 (9)
Mo3 <sup>v</sup> —Mo3—Mo2 <sup>vi</sup>	89.795 (12)	Se3 <sup>iii</sup> —Sc—Sc <sup>iii</sup>	110.81 (7)
Mo3 <sup>vi</sup> —Mo3—Mo2 <sup>vi</sup>	61.256 (13)	Se4 <sup>viii</sup> —Sc—Sc <sup>ii</sup>	49.97 (2)
Mo2 <sup>ix</sup> —Mo3—Mo2 <sup>vi</sup>	112.82 (2)	Se4—Sc—Sc <sup>ii</sup>	49.97 (2)
Se2 <sup>viii</sup> —Mo3—Mo2	145.46 (2)	Se3 <sup>ii</sup> —Sc—Sc <sup>ii</sup>	117.39 (6)
Se2—Mo3—Mo2	57.907 (12)	Se2 <sup>iii</sup> —Sc—Sc <sup>ii</sup>	114.00 (7)
Se3 <sup>v</sup> —Mo3—Mo2	60.350 (12)	Se2 <sup>xviii</sup> —Sc—Sc <sup>ii</sup>	114.00 (7)
Se3—Mo3—Mo2	118.538 (13)	Mo3 <sup>iii</sup> —Sc—Sc <sup>ii</sup>	103.78 (9)
Mo3 <sup>v</sup> —Mo3—Mo2	59.495 (13)	Se3 <sup>iii</sup> —Sc—Sc <sup>ii</sup>	50.81 (7)
Mo3 <sup>vi</sup> —Mo3—Mo2	88.794 (12)	Sc <sup>iii</sup> —Sc—Sc <sup>ii</sup>	60.0

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