

Na_{3.88}Mo₁₅Se₁₉: a novel ternary reduced molybdenum selenide containing Mo₆ and Mo₉ clusters

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Mo}-\text{Se}) = 0.001$ Å; disorder in solvent or counterion; R factor = 0.033; wR factor = 0.084; data-to-parameter ratio = 37.1.

The structure of tetrasodium pentadecamolybdenum nonadecaselenide, Na_{3.88}Mo₁₅Se₁₉, is isotopic with the In_{3+x}Mo₁₅Se₁₉ compounds [Grüttner *et al.* (1979). *Acta Cryst. B* **35**, 285–292]. It is characterized by two cluster units, Mo₆Seⁱ₈Se^a₆ and Mo₉Seⁱ₁₁Se^a₆ (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*b* and 2*c* and have point-group symmetry $\overline{3}$ and $\overline{6}$, respectively. The clusters are interconnected through additional Mo–Se bonds. In the title compound, the Na⁺ cations replace the trivalent as well as the monovalent indium atoms present in In_{3.9}Mo₁₅Se₁₉. One Mo, one Se and one Na atom are situated on mirror planes, and two other Se atoms and one Na atom [occupancy 0.628 (14)] are situated on threefold rotation axes. The crystal studied was twinned by merohedry with refined components of 0.4216 (12) and 0.5784 (12).

Related literature

For previous reports on the crystal structures of In₃Mo₁₅Se₁₉ compounds, see: Grüttner *et al.* (1979). For physical properties of this type of compounds, see: Seeber *et al.* (1979). The crystal structures of the substituted selenides Ho_{0.76}In_{1.68}Mo₁₅Se₁₉ and In_{0.87}K₂Mo₁₅Se₁₉ were reported by Salloum *et al.* (2006, 2007). For the isotopic sulfides In_{3.7}Mo₁₅S₁₉, In_{1.6}Rb₂Mo₁₅S₁₉, In_{2.2}CsMo₁₅S₁₉ and ScTl₂Mo₁₅S₁₉, see: Salloum *et al.* (2004a,b); Gougeon *et al.* (2010). For details of the *i*- and *a*-type ligand notation, see: Schäfer & von Schnerring (1964).

Experimental

Crystal data

Na _{3.88} Mo ₁₅ Se ₁₉	$Z = 2$
$M_r = 3028.54$	Mo $K\alpha$ radiation
Hexagonal, $P6_3/m$	$\mu = 26.47 \text{ mm}^{-1}$
$a = 9.8647 (1)$ Å	$T = 293$ K
$c = 19.5957 (3)$ Å	$0.09 \times 0.07 \times 0.06$ mm
$V = 1651.43 (3)$ Å ³	

Data collection

Nonius KappaCCD diffractometer	25999 measured reflections
Absorption correction: analytical (de Meulemaer & Tompa, 1965)	2487 independent reflections
$T_{\min} = 0.111$, $T_{\max} = 0.215$	2116 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.075$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$	67 parameters
$wR(F^2) = 0.084$	$\Delta\rho_{\max} = 2.69 \text{ e } \text{\AA}^{-3}$
$S = 1.06$	$\Delta\rho_{\min} = -1.81 \text{ e } \text{\AA}^{-3}$
2487 reflections	

Table 1
Selected bond lengths (Å).

Mo1–Se4 ⁱ	2.5287 (7)	Mo2–Mo3	2.7537 (6)
Mo1–Se1 ⁱⁱ	2.5600 (6)	Mo3–Se3	2.5586 (11)
Mo1–Se1	2.5810 (7)	Mo3–Se3 ^v	2.5675 (11)
Mo1–Se1 ⁱⁱⁱ	2.6075 (7)	Mo3–Se2	2.6153 (6)
Mo1–Mo1 ⁱⁱⁱ	2.6980 (7)	Mo3–Se2 ^{vii}	2.6153 (6)
Mo1–Mo1 ⁱⁱ	2.7152 (7)	Mo3–Mo3 ^{vi}	2.6834 (11)
Mo1–Se2 ^{iv}	2.7207 (7)	Se5–Na1	2.848 (6)
Mo2–Se5	2.5220 (7)	Na1–Se2 ^{viii}	3.2010 (11)
Mo2–Se2	2.6023 (8)	Na1–Se1 ^{ix}	3.462 (2)
Mo2–Mo2 ^v	2.6311 (7)	Na2–Se3 ^v	2.657 (5)
Mo2–Se2 ^{vi}	2.6312 (8)	Na2–Se4 ^{vii}	2.747 (4)
Mo2–Se3	2.6830 (6)	Na2–Se2 ^x	2.812 (4)
Mo2–Se1	2.7018 (7)	Na2–Se3 ^{xi}	3.096 (5)
Mo2–Mo3 ^{vi}	2.7153 (6)		

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

Data collection: COLLECT (Nonius, 1998); cell refinement: COLLECT; data reduction: EVALCCD (Duisenberg, 1998); program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHEXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Bergerhoff, 1996); software used to prepare material for publication: SHEXL97 and PLATON (Spek, 2009).

Intensity data were collected on the Nonius KappaCCD X-ray diffractometer system of the Centre de diffraction de l'Université de Rennes I (www.cdfx.univ-rennes1.fr).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2054).

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Na_{3.88}Mo₁₅Se₁₉: a novel ternary reduced molybdenum selenide containing Mo₆ and Mo₉ clusters

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S1. Comment

The reduced molybdenum compounds In_{3+x}Mo₁₅X₁₉ (X = S, Se) (Grüttner *et al.*, 1979; Salloum *et al.*, 2004a) crystallize in an interesting structural type characterized by an equal mixture of Mo₆ and Mo₉ clusters and by In atoms that occupy two or three different crystallographically positions depending on their formal oxidation state of +1 or +3. Subsequently, isomorphous compounds such as Ho_{0.76}In_{1.68}Mo₁₅Se₁₉ (Salloum *et al.*, 2006), In_{0.87}K₂Mo₁₅Se₁₉ (Salloum *et al.*, 2007), V_{1.42}In_{1.83}Mo₁₅Se₁₉ (Gougeon *et al.*, 2010), In_{3.7}Mo₁₅S₁₉ (Salloum *et al.*, 2004a), In_{1.6}Rb₂Mo₁₅S₁₉, In_{2.2}CsMo₁₅S₁₉ and ScTl₂Mo₁₅S₁₉ (Salloum *et al.*, 2004b) have been synthesized. In the latter compounds, the Ho, V and Sc atoms replace the trivalent indium and the K, Cs, and Tl atoms the monovalent one. We present here the crystal structure of Na_{3.9}Mo₁₅Se₁₉ in which the sodium replaces the monovalent as well as the trivalent indium for the first time.

The Mo—Se framework of the title compound consists of the cluster units Mo₆Seⁱ₈Se^a₆ and Mo₉Seⁱ₁₁Se^a₆ in a 1:1 ratio (for details of the i- and a-type ligand notation, see Schäfer & von Schnerring (1964)). Both components are interconnected through additional Mo—Se bonds (Figs. 1 and 2). The first unit can be described as an Mo₆ octahedron surrounded by eight face-capping inner Seⁱ and six apical Se^a ligands. The Mo₉ cluster is surrounded by 11 Seⁱ atoms capping one or two faces of the biotahedron and six Se^a ligands above the apical Mo atoms. The Mo₆Seⁱ₈Se^a₆ and Mo₉Seⁱ₁₁Se^a₆ units are centered at Wyckoff positions 2 b and 2c and have point-group symmetry $\bar{3}$ and $\bar{6}$, respectively. The Mo—Mo distances within the Mo₆ cluster are 2.6980 (7) Å for the distances of the Mo triangles formed by the Mo1 atoms related through the threefold axis, and 2.7152 (7) Å for the distances between these triangles. The Mo—Mo distances within the Mo₉ clusters are 2.6311 (7) and 2.6834 (11) Å in the triangles formed by the atoms Mo2 and Mo3, respectively, and 2.7153 (6) and 2.7537 (6) Å for those between the Mo₂ and Mo₃ 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 distances range from 2.5287 (7) to 2.7207 (7) Å within the Mo₆Seⁱ₈Se^a₆ unit, and from 2.5220 (7) to 2.7018 (7) Å within the Mo₉Seⁱ₁₁Se^a₆ unit. In both cases, the shortest bonds involve the Se4 and Se5 terminal atoms and the longest ones correspond to the interunit Mo1—Se2 and Mo2—Se1 bonds. Each Mo₉Seⁱ₁₁Se^a₆ cluster is thus interconnected to six Mo₆Seⁱ₈Se^a₆ units (and *vice versa*) via Mo2—Se1 bonds (and Mo1—Se2 bonds, respectively), forming the three-dimensional Mo—Se framework, the connective formula of which is Mo₉Seⁱ₅Se^a_{6/2}Seⁱ_{6/2}, Mo₆Seⁱ₂Se^a_{6/2}Seⁱ_{6/2}. It results from this arrangement that the shortest intercluster Mo1—Mo2 distance is 3.5202 (6) Å, indicating only weak metal-metal interactions between the Mo clusters. The Na⁺ cations are surrounded by seven Se atoms forming a distorted tricapped tetrahedron, as is the case in In_{3+x}Mo₁₅Se₁₉. The Se5 and Se2 atoms forming the tetrahedron are at 2.848 (6) and 3.2010 (11) Å from the Na1 atom, and the capping Se1 atoms are at 3.462 (2) Å. The Na2⁺ cations, as the In³⁺ cations in the In_{3.9}Mo₁₅Se₁₉ compounds, occupy partially at 62.7% a triangular group of distorted octahedral cavities around the threefold axis, which are formed by two Mo₆Seⁱ₈Se^a₆ and three

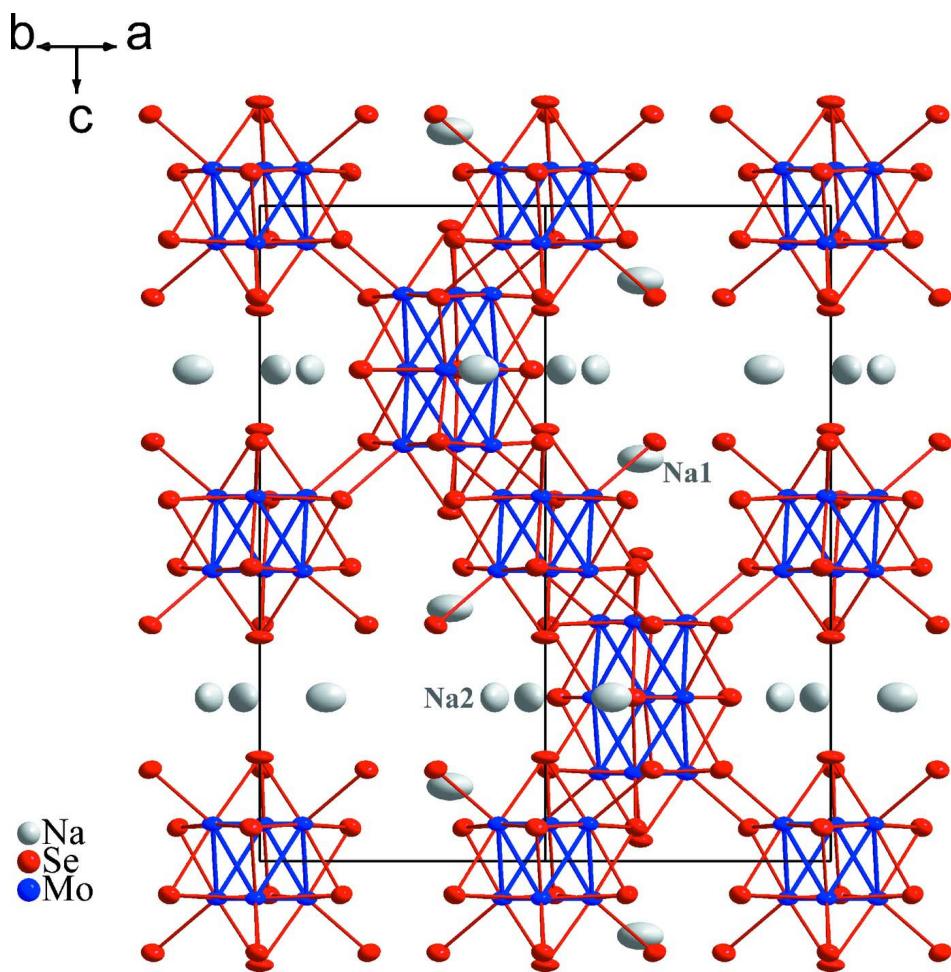
$\text{Mo}_9\text{Se}^{\text{i}}_{11}\text{Se}^{\text{a}}_6$ units. The Na2—Se distances are in the 2.657 (5) - 3.096 (5) Å range.

S2. Experimental

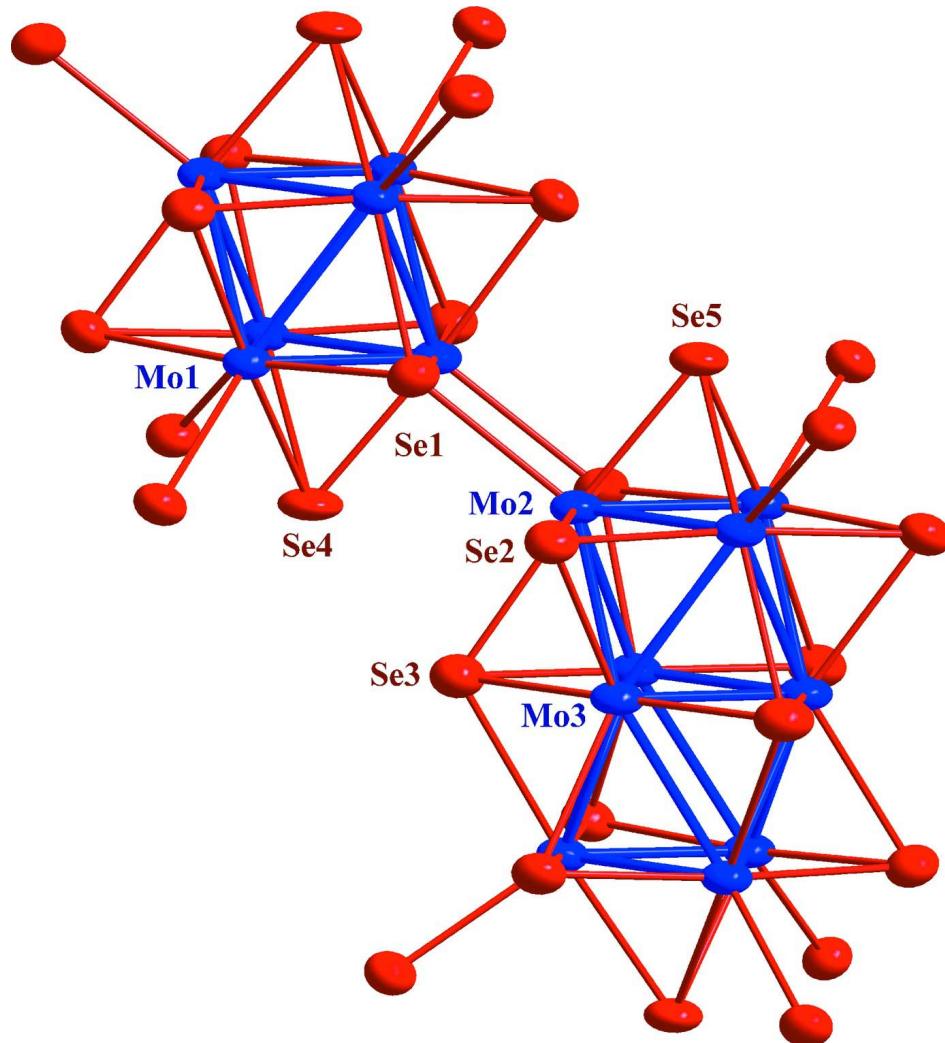
Single crystals of $\text{Na}_{3.9}\text{Mo}_{15}\text{Se}_{19}$ were prepared from an ion exchange reaction on single crystals of $\text{In}_{3+x}\text{Mo}_{15}\text{Se}_{19}$ with an excess of NaI at 1073 K. The mixture was sealed under vacuum in a long silica tube. The end of tube containing the crystals of $\text{In}_{3+x}\text{Mo}_{15}\text{Se}_{19}$ and InI was placed in a furnace with about 5 cm of the other end out from the furnace, at about the room temperature. The furnace was heated at 1073 K for 48 h. After reaction, crystals of InI were observed at the cool end of the tube. The black crystals of the title compound were subsequently washed with water to remove the excess of InI. Qualitative microanalyses using a Jeol JSM 6400 scanning electron microscope equipped with a Oxford INCA energy-dispersive-type X-ray spectrometer did not reveal the presence of indium in the crystals and indicated roughly stoichiometries comprised between 3.6 and 4.2 for the Na content.

S3. Refinement

Analysis of the intensity data using the TwinRotMat routine of *PLATON* (Spek, 2009) revealed the studied crystal was twinned by merohedry with $[110, 0\bar{1}0, 00\bar{1}]$ as the twin matrix. The ratio of the twin components was refined to 0.4216 (12):0.5784 (12). No significant deviation from full occupancy was observed for Na1. The site occupation factor of Na2 was refined freely leading to the final stoichiometry $\text{Na}_{3.88(4)}\text{Mo}_{15}\text{Se}_{19}$.

**Figure 1**

View of $\text{Na}_{3.9}\text{Mo}_{15}\text{Se}_{19}$ along [110]. Displacement ellipsoids are drawn at the 97% probability level.

**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.

Tetrasodium pentadecamolybdenum nonadecaselenide

Crystal data

$\text{Na}_{3.88}\text{Mo}_{15}\text{Se}_{19}$
 $M_r = 3028.54$
 Hexagonal, $P6_3/m$
 $a = 9.8647(1)$ Å
 $c = 19.5957(3)$ Å
 $V = 1651.43(3)$ Å³
 $Z = 2$
 $F(000) = 2637$

$D_x = 6.091 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
 Cell parameters from 26001 reflections
 $\theta = 1.7\text{--}35.0^\circ$
 $\mu = 26.47 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Multi-faceted crystal, black
 $0.09 \times 0.07 \times 0.06$ mm

Data collection

Nonius KappaCCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ scans ($\kappa = 0$) + additional ω scans
Absorption correction: analytical
(de Meulenaer & Tompa, 1965)
 $T_{\min} = 0.111$, $T_{\max} = 0.215$

25999 measured reflections
2487 independent reflections
2116 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.075$
 $\theta_{\max} = 35.0^\circ$, $\theta_{\min} = 2.4^\circ$
 $h = -15 \rightarrow 15$
 $k = -15 \rightarrow 15$
 $l = -19 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.084$
 $S = 1.06$
2487 reflections
67 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
 $w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 3.7236P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 2.69 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.81 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL*,
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00058 (8)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mo1	0.84973 (5)	-0.16457 (5)	0.556745 (19)	0.01378 (9)	
Mo2	0.68549 (6)	0.18962 (5)	0.63450 (2)	0.01510 (9)	
Mo3	0.51739 (7)	0.16952 (8)	0.7500	0.01574 (11)	
Se1	0.68259 (6)	-0.03045 (6)	0.55145 (2)	0.01653 (11)	
Se2	0.38303 (7)	0.00893 (7)	0.63968 (2)	0.01760 (11)	
Se3	0.69343 (10)	0.04771 (10)	0.7500	0.01993 (16)	
Se4	0.0000	0.0000	0.65840 (4)	0.0222 (2)	
Se5	0.6667	0.3333	0.53176 (4)	0.01851 (18)	
Na1	0.6667	0.3333	0.3864 (3)	0.0618 (18)	
Na2	0.0558 (6)	0.2330 (7)	0.7500	0.0214 (16)	0.628 (14)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.01667 (19)	0.01711 (19)	0.00794 (16)	0.00872 (17)	0.00032 (12)	0.00005 (13)
Mo2	0.0186 (2)	0.0185 (2)	0.00811 (15)	0.00916 (17)	-0.00004 (14)	-0.00039 (13)

Mo3	0.0195 (3)	0.0198 (3)	0.0079 (2)	0.0097 (2)	0.000	0.000
Se1	0.0181 (2)	0.0198 (3)	0.01279 (19)	0.0103 (2)	0.00148 (17)	-0.00079 (17)
Se2	0.0198 (2)	0.0200 (2)	0.01247 (19)	0.0095 (2)	-0.00268 (17)	-0.00173 (17)
Se3	0.0252 (4)	0.0232 (4)	0.0131 (3)	0.0134 (3)	0.000	0.000
Se4	0.0297 (3)	0.0297 (3)	0.0071 (3)	0.01486 (15)	0.000	0.000
Se5	0.0239 (3)	0.0239 (3)	0.0078 (3)	0.01194 (14)	0.000	0.000
Na1	0.079 (3)	0.079 (3)	0.028 (3)	0.0393 (15)	0.000	0.000
Na2	0.017 (3)	0.035 (3)	0.019 (2)	0.018 (2)	0.000	0.000

Geometric parameters (\AA , ^\circ)

Mo1—Se4 ⁱ	2.5287 (7)	Se1—Na1 ^{xiii}	3.462 (2)
Mo1—Se1 ⁱⁱ	2.5600 (6)	Se2—Mo2 ^{ix}	2.6312 (8)
Mo1—Se1	2.5810 (7)	Se2—Mo1 ^{xiv}	2.7207 (7)
Mo1—Se1 ⁱⁱⁱ	2.6075 (7)	Se2—Na2 ^{xii}	2.812 (4)
Mo1—Mo1 ⁱⁱⁱ	2.6980 (7)	Se2—Na1 ^{xiii}	3.2010 (11)
Mo1—Mo1 ^{iv}	2.6980 (7)	Se3—Mo3 ^{viii}	2.5675 (11)
Mo1—Mo1 ⁱⁱ	2.7152 (7)	Se3—Na2 ^{viii}	2.657 (5)
Mo1—Mo1 ^v	2.7152 (7)	Se3—Mo2 ^x	2.6830 (6)
Mo1—Se2 ^{vi}	2.7207 (7)	Se3—Na2 ⁱ	3.096 (5)
Mo1—Mo2 ⁱⁱⁱ	3.5202 (6)	Se4—Mo1 ^{xv}	2.5287 (7)
Mo1—Mo1 ^{vii}	3.8278 (8)	Se4—Mo1 ^{xiv}	2.5287 (7)
Mo1—Na2 ^{viii}	3.8628 (12)	Se4—Mo1 ^{ix}	2.5287 (7)
Mo2—Se5	2.5220 (7)	Se4—Na2 ^{xii}	2.747 (4)
Mo2—Se2	2.6023 (8)	Se4—Na2	2.747 (4)
Mo2—Mo2 ^{ix}	2.6311 (7)	Se4—Na2 ^{xvi}	2.747 (5)
Mo2—Mo2 ^{viii}	2.6311 (7)	Se5—Mo2 ^{viii}	2.5220 (7)
Mo2—Se2 ^{viii}	2.6312 (8)	Se5—Mo2 ^{ix}	2.5220 (7)
Mo2—Se3	2.6830 (6)	Se5—Na1	2.848 (6)
Mo2—Se1	2.7018 (7)	Na1—Se2 ^{xiii}	3.2010 (11)
Mo2—Mo3 ^{viii}	2.7153 (6)	Na1—Se2 ^v	3.2010 (11)
Mo2—Mo3	2.7537 (6)	Na1—Se2 ^{xvii}	3.2010 (11)
Mo2—Mo1 ^{iv}	3.5202 (6)	Na1—Se1 ^v	3.462 (2)
Mo3—Se3	2.5586 (11)	Na1—Se1 ^{xiii}	3.462 (2)
Mo3—Se3 ^{ix}	2.5675 (11)	Na1—Se1 ^{xvii}	3.462 (2)
Mo3—Se2	2.6153 (6)	Na2—Se3 ^{ix}	2.657 (5)
Mo3—Se2 ^x	2.6153 (6)	Na2—Se4 ^x	2.747 (4)
Mo3—Mo3 ^{viii}	2.6834 (11)	Na2—Se2 ^{xviii}	2.812 (4)
Mo3—Mo3 ^{ix}	2.6834 (11)	Na2—Se2 ^{xvi}	2.812 (4)
Mo3—Mo2 ^{xi}	2.7153 (6)	Na2—Mo3 ^{xvi}	2.956 (5)
Mo3—Mo2 ^{ix}	2.7153 (6)	Na2—Se3 ^{xv}	3.096 (5)
Mo3—Mo2 ^x	2.7537 (6)	Na2—Na2 ^{xvi}	3.601 (10)
Mo3—Na2 ^{xii}	2.956 (5)	Na2—Na2 ^{xii}	3.601 (10)
Se1—Mo1 ^v	2.5600 (6)	Na2—Mo1 ^{xi}	3.8628 (12)
Se1—Mo1 ^{iv}	2.6075 (7)	Na2—Mo1 ^{ix}	3.8628 (12)
Se4 ⁱ —Mo1—Se1 ⁱⁱ	176.02 (2)	Mo3 ^{ix} —Mo3—Mo2	89.039 (15)
Se4 ⁱ —Mo1—Se1	91.274 (18)	Mo2 ^{xi} —Mo3—Mo2	146.42 (3)

Se1 ⁱⁱ —Mo1—Se1	89.153 (17)	Mo2 ^{ix} —Mo3—Mo2	57.508 (17)
Se4 ⁱ —Mo1—Se1 ⁱⁱⁱ	90.664 (18)	Mo2 ^x —Mo3—Mo2	110.55 (3)
Se1 ⁱⁱ —Mo1—Se1 ⁱⁱⁱ	88.572 (18)	Se3—Mo3—Na2 ^{xii}	115.38 (12)
Se1—Mo1—Se1 ⁱⁱⁱ	174.67 (3)	Se3 ^{ix} —Mo3—Na2 ^{xii}	67.75 (12)
Se4 ⁱ —Mo1—Mo1 ⁱⁱⁱ	57.759 (12)	Se2—Mo3—Na2 ^{xii}	60.24 (4)
Se1 ⁱⁱ —Mo1—Mo1 ⁱⁱⁱ	118.706 (18)	Se2 ^x —Mo3—Na2 ^{xii}	60.24 (4)
Se1—Mo1—Mo1 ⁱⁱⁱ	119.10 (2)	Mo3 ^{viii} —Mo3—Na2 ^{xii}	173.98 (12)
Se1 ⁱⁱⁱ —Mo1—Mo1 ⁱⁱⁱ	58.19 (2)	Mo3 ^{ix} —Mo3—Na2 ^{xii}	126.02 (12)
Se4 ⁱ —Mo1—Mo1 ^{iv}	57.759 (12)	Mo2 ^{xi} —Mo3—Na2 ^{xii}	93.47 (6)
Se1 ⁱⁱ —Mo1—Mo1 ^{iv}	119.357 (19)	Mo2 ^{ix} —Mo3—Na2 ^{xii}	93.47 (6)
Se1—Mo1—Mo1 ^{iv}	59.15 (2)	Mo2 ^x —Mo3—Na2 ^{xii}	118.06 (4)
Se1 ⁱⁱⁱ —Mo1—Mo1 ^{iv}	118.14 (2)	Mo2—Mo3—Na2 ^{xii}	118.06 (4)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^{iv}	60.0	Mo1 ^v —Se1—Mo1	63.76 (2)
Se4 ⁱ —Mo1—Mo1 ⁱⁱ	117.937 (16)	Mo1 ^v —Se1—Mo1 ^{iv}	63.39 (2)
Se1 ⁱⁱ —Mo1—Mo1 ⁱⁱ	58.50 (2)	Mo1—Se1—Mo1 ^{iv}	62.66 (2)
Se1—Mo1—Mo1 ⁱⁱ	117.326 (19)	Mo1 ^v —Se1—Mo2	132.81 (3)
Se1 ⁱⁱⁱ —Mo1—Mo1 ⁱⁱ	57.453 (14)	Mo1—Se1—Mo2	129.41 (2)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ⁱⁱ	60.209 (10)	Mo1 ^{iv} —Se1—Mo2	83.04 (2)
Mo1 ^{iv} —Mo1—Mo1 ⁱⁱ	90.0	Mo1 ^v —Se1—Na1 ^{xiii}	130.23 (8)
Se4 ⁱ —Mo1—Mo1 ^v	117.937 (16)	Mo1—Se1—Na1 ^{xiii}	99.13 (2)
Se1 ⁱⁱ —Mo1—Mo1 ^v	59.16 (2)	Mo1 ^{iv} —Se1—Na1 ^{xiii}	151.91 (7)
Se1—Mo1—Mo1 ^v	57.743 (15)	Mo2—Se1—Na1 ^{xiii}	95.04 (6)
Se1 ⁱⁱⁱ —Mo1—Mo1 ^v	117.026 (19)	Mo2—Se2—Mo3	63.71 (2)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^v	90.0	Mo2—Se2—Mo2 ^{ix}	60.36 (2)
Mo1 ^{iv} —Mo1—Mo1 ^v	60.209 (9)	Mo3—Se2—Mo2 ^{ix}	62.333 (19)
Mo1 ⁱⁱ —Mo1—Mo1 ^v	59.583 (19)	Mo2—Se2—Mo1 ^{xiv}	127.69 (2)
Se4 ⁱ —Mo1—Se2 ^{vi}	91.21 (2)	Mo3—Se2—Mo1 ^{xiv}	130.42 (3)
Se1 ⁱⁱ —Mo1—Se2 ^{vi}	92.77 (2)	Mo2 ^{ix} —Se2—Mo1 ^{xiv}	82.24 (2)
Se1—Mo1—Se2 ^{vi}	87.51 (2)	Mo2—Se2—Na2 ^{xii}	129.48 (9)
Se1 ⁱⁱⁱ —Mo1—Se2 ^{vi}	97.41 (2)	Mo3—Se2—Na2 ^{xii}	65.90 (8)
Mo1 ⁱⁱⁱ —Mo1—Se2 ^{vi}	136.97 (2)	Mo2 ^{ix} —Se2—Na2 ^{xii}	98.77 (11)
Mo1 ^{iv} —Mo1—Se2 ^{vi}	130.63 (2)	Mo1 ^{xiv} —Se2—Na2 ^{xii}	88.56 (10)
Mo1 ⁱⁱ —Mo1—Se2 ^{vi}	139.27 (2)	Mo2—Se2—Na1 ^{xiii}	103.57 (2)
Mo1 ^v —Mo1—Se2 ^{vi}	132.73 (2)	Mo3—Se2—Na1 ^{xiii}	122.35 (10)
Se4 ⁱ —Mo1—Mo2 ⁱⁱⁱ	91.163 (16)	Mo2 ^{ix} —Se2—Na1 ^{xiii}	160.83 (7)
Se1 ⁱⁱ —Mo1—Mo2 ⁱⁱⁱ	91.320 (19)	Mo1 ^{xiv} —Se2—Na1 ^{xiii}	102.71 (7)
Se1—Mo1—Mo2 ⁱⁱⁱ	135.27 (2)	Na2 ^{xii} —Se2—Na1 ^{xiii}	99.85 (14)
Se1 ⁱⁱⁱ —Mo1—Mo2 ⁱⁱⁱ	49.629 (15)	Mo3—Se3—Mo3 ^{viii}	63.13 (3)
Mo1 ⁱⁱⁱ —Mo1—Mo2 ⁱⁱⁱ	99.53 (2)	Mo3—Se3—Na2 ^{viii}	157.67 (13)
Mo1 ^{iv} —Mo1—Mo2 ⁱⁱⁱ	148.233 (15)	Mo3 ^{viii} —Se3—Na2 ^{viii}	139.20 (13)
Mo1 ⁱⁱ —Mo1—Mo2 ⁱⁱⁱ	100.519 (16)	Mo3—Se3—Mo2 ^x	63.33 (2)
Mo1 ^v —Mo1—Mo2 ⁱⁱⁱ	149.644 (19)	Mo3 ^{viii} —Se3—Mo2 ^x	62.236 (19)
Se2 ^{vi} —Mo1—Mo2 ⁱⁱⁱ	47.784 (15)	Na2 ^{viii} —Se3—Mo2 ^x	121.81 (2)
Se4 ⁱ —Mo1—Mo1 ^{vii}	87.495 (19)	Mo3—Se3—Mo2	63.33 (2)
Se1 ⁱⁱ —Mo1—Mo1 ^{vii}	88.562 (18)	Mo3 ^{viii} —Se3—Mo2	62.236 (19)
Se1—Mo1—Mo1 ^{vii}	87.95 (2)	Na2 ^{viii} —Se3—Mo2	121.81 (2)
Se1 ⁱⁱⁱ —Mo1—Mo1 ^{vii}	87.18 (2)	Mo2 ^x —Se3—Mo2	115.04 (3)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^{vii}	45.181 (8)	Mo3—Se3—Na2 ⁱ	125.24 (11)

Mo1 ^{iv} —Mo1—Mo1 ^{vii}	45.181 (8)	Mo3 ^{viii} —Se3—Na2 ⁱ	62.11 (11)
Mo1 ⁱⁱ —Mo1—Mo1 ^{vii}	44.819 (8)	Na2 ^{viii} —Se3—Na2 ⁱ	77.1 (2)
Mo1 ^v —Mo1—Mo1 ^{vii}	44.819 (8)	Mo2 ^x —Se3—Na2 ⁱ	91.04 (6)
Se2 ^{vi} —Mo1—Mo1 ^{vii}	175.25 (3)	Mo2—Se3—Na2 ⁱ	91.04 (6)
Mo2 ⁱⁱⁱ —Mo1—Mo1 ^{vii}	136.78 (2)	Mo1 ^{xv} —Se4—Mo1 ^{xiv}	64.48 (2)
Se4 ⁱ —Mo1—Na2 ^{viii}	45.18 (9)	Mo1 ^{xv} —Se4—Mo1 ^{ix}	64.48 (2)
Se1 ⁱⁱ —Mo1—Na2 ^{viii}	138.79 (9)	Mo1 ^{xiv} —Se4—Mo1 ^{ix}	64.48 (2)
Se1—Mo1—Na2 ^{viii}	82.95 (8)	Mo1 ^{xv} —Se4—Na2 ^{xii}	127.86 (10)
Se1 ⁱⁱⁱ —Mo1—Na2 ^{viii}	101.91 (8)	Mo1 ^{xiv} —Se4—Na2 ^{xii}	94.05 (8)
Mo1 ⁱⁱⁱ —Mo1—Na2 ^{viii}	100.18 (9)	Mo1 ^{ix} —Se4—Na2 ^{xii}	149.31 (10)
Mo1 ^{iv} —Mo1—Na2 ^{viii}	90.73 (8)	Mo1 ^{xv} —Se4—Na2	149.31 (9)
Mo1 ⁱⁱ —Mo1—Na2 ^{viii}	156.33 (8)	Mo1 ^{xiv} —Se4—Na2	127.86 (10)
Mo1 ^v —Mo1—Na2 ^{viii}	138.84 (7)	Mo1 ^{ix} —Se4—Na2	94.05 (8)
Se2 ^{vi} —Mo1—Na2 ^{viii}	46.69 (8)	Na2 ^{xii} —Se4—Na2	81.92 (12)
Mo2 ⁱⁱⁱ —Mo1—Na2 ^{viii}	67.91 (7)	Mo1 ^{xv} —Se4—Na2 ^{xvi}	94.05 (8)
Mo1 ^{vii} —Mo1—Na2 ^{viii}	131.19 (9)	Mo1 ^{xiv} —Se4—Na2 ^{xvi}	149.31 (9)
Se5—Mo2—Se2	91.991 (19)	Mo1 ^{ix} —Se4—Na2 ^{xvi}	127.86 (10)
Se5—Mo2—Mo2 ^{ix}	58.558 (12)	Na2 ^{xii} —Se4—Na2 ^{xvi}	81.92 (12)
Se2—Mo2—Mo2 ^{ix}	60.37 (3)	Na2—Se4—Na2 ^{xvi}	81.92 (12)
Se5—Mo2—Mo2 ^{viii}	58.558 (12)	Mo2 ^{viii} —Se5—Mo2	62.88 (2)
Se2—Mo2—Mo2 ^{viii}	120.31 (3)	Mo2 ^{viii} —Se5—Mo2 ^{ix}	62.88 (2)
Mo2 ^{ix} —Mo2—Mo2 ^{viii}	60.0	Mo2—Se5—Mo2 ^{ix}	62.88 (2)
Se5—Mo2—Se2 ^{viii}	91.314 (18)	Mo2 ^{viii} —Se5—Na1	142.963 (15)
Se2—Mo2—Se2 ^{viii}	175.53 (3)	Mo2—Se5—Na1	142.963 (15)
Mo2 ^{ix} —Mo2—Se2 ^{viii}	119.22 (2)	Mo2 ^{ix} —Se5—Na1	142.963 (15)
Mo2 ^{viii} —Mo2—Se2 ^{viii}	59.27 (2)	Se5—Na1—Se2 ^{xiii}	99.20 (10)
Se5—Mo2—Se3	175.05 (3)	Se5—Na1—Se2 ^v	99.20 (10)
Se2—Mo2—Se3	86.12 (2)	Se2 ^{xiii} —Na1—Se2 ^v	117.49 (6)
Mo2 ^{ix} —Mo2—Se3	116.64 (2)	Se5—Na1—Se2 ^{xvii}	99.20 (10)
Mo2 ^{viii} —Mo2—Se3	118.69 (2)	Se2 ^{xiii} —Na1—Se2 ^{xvii}	117.49 (6)
Se2 ^{viii} —Mo2—Se3	90.35 (3)	Se2 ^v —Na1—Se2 ^{xvii}	117.49 (6)
Se5—Mo2—Se1	89.81 (2)	Se5—Na1—Se1 ^v	69.42 (9)
Se2—Mo2—Se1	85.71 (2)	Se2 ^{xiii} —Na1—Se1 ^v	66.67 (2)
Mo2 ^{ix} —Mo2—Se1	129.77 (2)	Se2 ^v —Na1—Se1 ^v	65.44 (2)
Mo2 ^{viii} —Mo2—Se1	137.17 (2)	Se2 ^{xvii} —Na1—Se1 ^v	168.60 (19)
Se2 ^{viii} —Mo2—Se1	97.31 (2)	Se5—Na1—Se1 ^{xiii}	69.42 (9)
Se3—Mo2—Se1	94.60 (2)	Se2 ^{xiii} —Na1—Se1 ^{xiii}	65.44 (2)
Se5—Mo2—Mo3 ^{viii}	120.52 (2)	Se2 ^v —Na1—Se1 ^{xiii}	168.60 (19)
Se2—Mo2—Mo3 ^{viii}	117.08 (2)	Se2 ^{xvii} —Na1—Se1 ^{xiii}	66.67 (2)
Mo2 ^{ix} —Mo2—Mo3 ^{viii}	90.964 (15)	Se1 ^v —Na1—Se1 ^{xiii}	108.34 (9)
Mo2 ^{viii} —Mo2—Mo3 ^{viii}	61.980 (17)	Se5—Na1—Se1 ^{xvii}	69.42 (9)
Se2 ^{viii} —Mo2—Mo3 ^{viii}	58.547 (18)	Se2 ^{xiii} —Na1—Se1 ^{xvii}	168.60 (19)
Se3—Mo2—Mo3 ^{viii}	56.80 (2)	Se2 ^v —Na1—Se1 ^{xvii}	66.67 (2)
Se1—Mo2—Mo3 ^{viii}	139.02 (2)	Se2 ^{xvii} —Na1—Se1 ^{xvii}	65.44 (2)
Se5—Mo2—Mo3	119.05 (2)	Se1 ^v —Na1—Se1 ^{xvii}	108.34 (9)
Se2—Mo2—Mo3	58.376 (18)	Se1 ^{xiii} —Na1—Se1 ^{xvii}	108.34 (9)
Mo2 ^{ix} —Mo2—Mo3	60.511 (18)	Se3 ^{ix} —Na2—Se4	87.67 (13)
Mo2 ^{viii} —Mo2—Mo3	90.119 (16)	Se3 ^{ix} —Na2—Se4 ^x	87.67 (13)

Se2 ^{viii} —Mo2—Mo3	117.29 (2)	Se4—Na2—Se4 ^x	81.61 (16)
Se3—Mo2—Mo3	56.13 (2)	Se3 ^{ix} —Na2—Se2 ^{xviii}	111.08 (14)
Se1—Mo2—Mo3	132.31 (2)	Se4—Na2—Se2 ^{xviii}	156.4 (2)
Mo3 ^{viii} —Mo2—Mo3	58.76 (2)	Se4 ^x —Na2—Se2 ^{xviii}	84.93 (4)
Se5—Mo2—Mo1 ^{iv}	91.085 (16)	Se3 ^{ix} —Na2—Se2 ^{xvi}	111.08 (14)
Se2—Mo2—Mo1 ^{iv}	132.93 (2)	Se4—Na2—Se2 ^{xvi}	84.93 (4)
Mo2 ^{ix} —Mo2—Mo1 ^{iv}	149.106 (14)	Se4 ^x —Na2—Se2 ^{xvi}	156.4 (2)
Mo2 ^{viii} —Mo2—Mo1 ^{iv}	100.94 (2)	Se2 ^{xviii} —Na2—Se2 ^{xvi}	100.51 (17)
Se2 ^{viii} —Mo2—Mo1 ^{iv}	49.978 (15)	Se3 ^{ix} —Na2—Mo3 ^{xvi}	146.9 (2)
Se3—Mo2—Mo1 ^{iv}	93.55 (2)	Se4—Na2—Mo3 ^{xvi}	116.51 (14)
Se1—Mo2—Mo1 ^{iv}	47.329 (15)	Se4 ^x —Na2—Mo3 ^{xvi}	116.51 (14)
Mo3 ^{viii} —Mo2—Mo1 ^{iv}	101.18 (2)	Se2 ^{xviii} —Na2—Mo3 ^{xvi}	53.86 (9)
Mo3—Mo2—Mo1 ^{iv}	149.02 (2)	Se2 ^{xvi} —Na2—Mo3 ^{xvi}	53.86 (9)
Se3—Mo3—Se3 ^{ix}	176.87 (3)	Se3 ^{ix} —Na2—Se3 ^{xv}	162.9 (2)
Se3—Mo3—Se2	88.45 (2)	Se4—Na2—Se3 ^{xv}	79.44 (13)
Se3 ^{ix} —Mo3—Se2	93.31 (2)	Se4 ^x —Na2—Se3 ^{xv}	79.44 (13)
Se3—Mo3—Se2 ^x	88.45 (2)	Se2 ^{xviii} —Na2—Se3 ^{xv}	79.14 (11)
Se3 ^{ix} —Mo3—Se2 ^x	93.31 (2)	Se2 ^{xvi} —Na2—Se3 ^{xv}	79.14 (11)
Se2—Mo3—Se2 ^x	111.50 (3)	Mo3 ^{xvi} —Na2—Se3 ^{xv}	50.14 (8)
Se3—Mo3—Mo3 ^{viii}	58.60 (4)	Se3 ^{ix} —Na2—Na2 ^{xvi}	116.92 (17)
Se3 ^{ix} —Mo3—Mo3 ^{viii}	118.27 (4)	Se4—Na2—Na2 ^{xvi}	49.04 (6)
Se2—Mo3—Mo3 ^{viii}	117.76 (2)	Se4 ^x —Na2—Na2 ^{xvi}	49.04 (6)
Se2 ^x —Mo3—Mo3 ^{viii}	117.76 (2)	Se2 ^{xviii} —Na2—Na2 ^{xvi}	107.97 (17)
Se3—Mo3—Mo3 ^{ix}	118.60 (3)	Se2 ^{xvi} —Na2—Na2 ^{xvi}	107.97 (17)
Se3 ^{ix} —Mo3—Mo3 ^{ix}	58.27 (4)	Mo3 ^{xvi} —Na2—Na2 ^{xvi}	96.1 (2)
Se2—Mo3—Mo3 ^{ix}	120.43 (2)	Se3 ^{xv} —Na2—Na2 ^{xvi}	45.99 (16)
Se2 ^x —Mo3—Mo3 ^{ix}	120.43 (2)	Se3 ^{ix} —Na2—Na2 ^{xii}	56.92 (17)
Mo3 ^{viii} —Mo3—Mo3 ^{ix}	60.0	Se4—Na2—Na2 ^{xii}	49.04 (6)
Se3—Mo3—Mo2 ^{xi}	118.045 (18)	Se4 ^x —Na2—Na2 ^{xii}	49.04 (6)
Se3 ^{ix} —Mo3—Mo2 ^{xi}	60.968 (17)	Se2 ^{xviii} —Na2—Na2 ^{xii}	129.74 (9)
Se2—Mo3—Mo2 ^{xi}	149.86 (3)	Se2 ^{xvi} —Na2—Na2 ^{xii}	129.74 (9)
Se2 ^x —Mo3—Mo2 ^{xi}	59.121 (17)	Mo3 ^{xvi} —Na2—Na2 ^{xii}	156.1 (2)
Mo3 ^{viii} —Mo3—Mo2 ^{xi}	89.853 (16)	Se3 ^{xv} —Na2—Na2 ^{xii}	105.99 (16)
Mo3 ^{ix} —Mo3—Mo2 ^{xi}	61.335 (19)	Na2 ^{xvi} —Na2—Na2 ^{xii}	60.000 (1)
Se3—Mo3—Mo2 ^{ix}	118.045 (18)	Se3 ^{ix} —Na2—Mo1 ^{xi}	96.57 (7)
Se3 ^{ix} —Mo3—Mo2 ^{ix}	60.968 (17)	Se4—Na2—Mo1 ^{xi}	121.60 (17)
Se2—Mo3—Mo2 ^{ix}	59.121 (17)	Se4 ^x —Na2—Mo1 ^{xi}	40.767 (18)
Se2 ^x —Mo3—Mo2 ^{ix}	149.86 (3)	Se2 ^{xviii} —Na2—Mo1 ^{xi}	44.758 (19)
Mo3 ^{viii} —Mo3—Mo2 ^{ix}	89.853 (16)	Se2 ^{xvi} —Na2—Mo1 ^{xi}	142.89 (16)
Mo3 ^{ix} —Mo3—Mo2 ^{ix}	61.335 (19)	Mo3 ^{xvi} —Na2—Mo1 ^{xi}	89.52 (8)
Mo2 ^{xi} —Mo3—Mo2 ^{ix}	112.93 (3)	Se3 ^{xv} —Na2—Mo1 ^{xi}	80.99 (8)
Se3—Mo3—Mo2 ^x	60.536 (17)	Na2 ^{xvi} —Na2—Mo1 ^{xi}	78.76 (9)
Se3 ^{ix} —Mo3—Mo2 ^x	118.389 (19)	Na2 ^{xii} —Na2—Mo1 ^{xi}	85.87 (7)
Se2—Mo3—Mo2 ^x	145.85 (3)	Se3 ^{ix} —Na2—Mo1 ^{ix}	96.57 (7)
Se2 ^x —Mo3—Mo2 ^x	57.914 (17)	Se4—Na2—Mo1 ^{ix}	40.767 (18)
Mo3 ^{viii} —Mo3—Mo2 ^x	59.903 (18)	Se4 ^x —Na2—Mo1 ^{ix}	121.60 (17)
Mo3 ^{ix} —Mo3—Mo2 ^x	89.039 (15)	Se2 ^{xviii} —Na2—Mo1 ^{ix}	142.89 (16)
Mo2 ^{xi} —Mo3—Mo2 ^x	57.509 (17)	Se2 ^{xvi} —Na2—Mo1 ^{ix}	44.758 (19)

Mo2 ^{ix} —Mo3—Mo2 ^x	146.42 (3)	Mo3 ^{xvi} —Na2—Mo1 ^{ix}	89.52 (8)
Se3—Mo3—Mo2	60.536 (17)	Se3 ^{xv} —Na2—Mo1 ^{ix}	80.99 (8)
Se3 ^{ix} —Mo3—Mo2	118.388 (19)	Na2 ^{xvi} —Na2—Mo1 ^{ix}	78.76 (9)
Se2—Mo3—Mo2	57.913 (17)	Na2 ^{xii} —Na2—Mo1 ^{ix}	85.87 (7)
Se2 ^x —Mo3—Mo2	145.85 (3)	Mo1 ^{xi} —Na2—Mo1 ^{ix}	157.26 (17)
Mo3 ^{viii} —Mo3—Mo2	59.903 (18)		

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