Tetra-μ_3-selenido-1:2:3κ^3Se;1:2:4κ^3Se;1:3:4κ^3Se;-2:3:4κ^3Se-tetrakis[(η^5-methylcyclopentadienyl)-molybdenum(III)](6 *Mo—Mo*)

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The title cluster compound, [Mo$_4$(η^5-C$_5$H$_4$Me)$_4$(μ_3-Se)$_4$], was synthesized from the reaction of [Mo(η^5-C$_5$H$_4$Me)(CO)$_3$]$_2$ with grey selenium in refluxing xylene solution under a nitrogen atmosphere. The complete cluster is generated by a crystallographic twofold axis and contains an Mo$_4$Se$_4$ cubane-like core surrounded by four η^5-methylcyclopentadienyl ligands. In the core, the four molybdenum atoms are connected to each other to form a tetrahedron, with a selenium atom capping each face. The Mo—Mo bond lengths vary from 2.9857 (5) to 3.0083 (3) Å and the Mo—Se separations range from 2.4633 (4) to 2.4693 (5) Å.

3D view

Chemical scheme
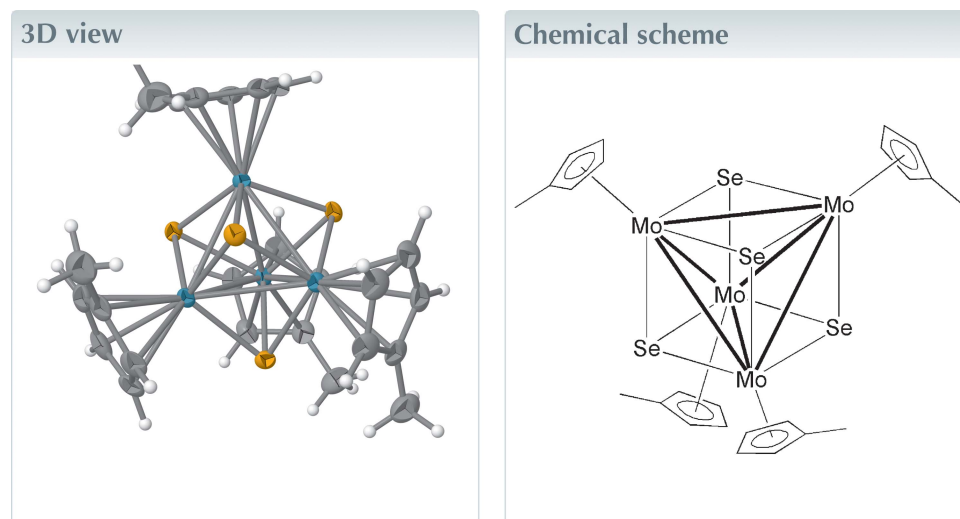
Structure description

In comparison to many studies on transition-metal sulfur cubane-type clusters, which contain an M_4S$_4$ core, those on selenium analogues are relatively rare. One of the reasons for this rarity could be caused by the insolubility of grey selenium to common organic solvents, as well as water, which are employed for synthesis. We found that grey selenium easily reacts with the organometallic molybdenum compound [Mo(η^5-C$_5$H$_4$Me)(CO)$_3$]$_2$ in organic media to produce a new molybdenum-selenium cubane-type cluster [Mo$_4$(η^5-C$_5$H$_4$Me)$_4$(μ_3-Se)$_4$]. We now report the structural details of the cluster. The partially labeled molecular structure of the title compound is shown in Fig. 1. The cluster possess twofold symmetry because of the existence of twofold axis through the cluster. The cluster has a distorted-cubane type Mo$_4$Se$_4$ core surrounded by four methylcyclopentadienyl ligands. In the core, four molybdenum atoms are connected by each other through six Mo—Mo bonds to give a molybdenum tetrahedron. The distances of the Mo—Mo bonds range from 2.9857 (5) to 3.0083 (3) Å, which are somewhat longer than those in
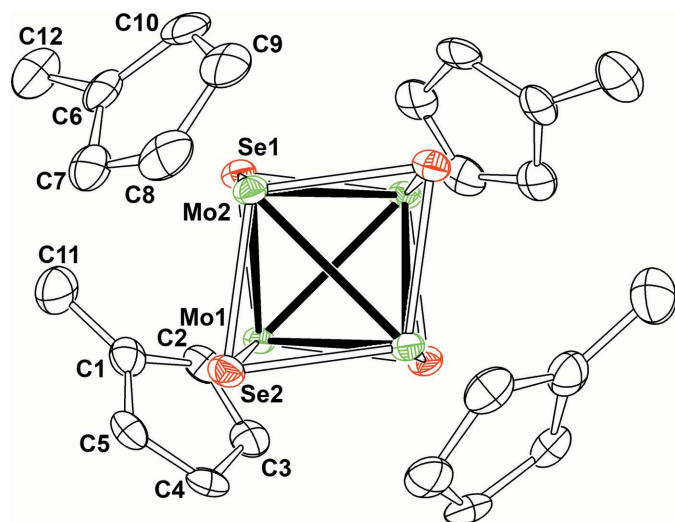
Figure 1
A view of the molecular structure of the title compound, with the asymmetric atoms labeled; unlabelled atoms are generated by the symmetry operation $-x, y, \frac{3}{2} - z$. Hydrogen atoms are omitted for charity. Displacement ellipsoids are drawn at the 50% probability level.

$[Mo_4(H_2O)_{12}(\mu_3\text{-}Se)_4](MeC_6H_4SO_3)_5 \cdot 15H_2O$ [mean value 2.865 (4) Å; Henkel *et al.*, 1990] and $(NH_4)_6[Mo_4(CN)_{12}(\mu_3\text{-}Se)_4]\cdot 6H_2O$ [2.886 (4) Å, T_d symmetry; Virovets *et al.*, 2000]. However, the Mo—Mo distances in the title compound are quite close to those in an isoelectronic cluster $[Mo_4(\eta^5\text{-}C_5H_4Pr^i)_4(\mu_3\text{-}Se)_4]$ (mean value of 2.9870 Å), which was synthesized by the reaction of $[Mo_2(\eta^5\text{-}C_5H_4Pr^i)_2(\mu\text{-}Cl)_4]$ with LiSeH (Baird *et al.*, 1991). On each face of the Mo tetrahedron, a selenium atom is located. The Mo—Se distances are in the range 2.4633 (4) to 2.4693 (5) Å and are normal.

Synthesis and crystallization

A xylene solution (30 ml) of $[Mo(\eta^5\text{-}C_5H_4Me)(CO)_3]_2$ (519 mg, 1.00 mmol) and grey selenium (180 mg, 2.28 mmol) was refluxed for 17 h under a nitrogen atmosphere. The color of the solution gradually changed from red to brown. After removal of excess selenium by filtration, evaporation of the solvent from the filtrate gave a purple–brown solid. Crystallization was performed by use of the mixed solvents $CH_2Cl_2/$ diethyl ether (1:2 *v/v*). Yield: 300 mg (59%). A single-crystal suitable for X-ray analysis was selected from the crystallized sample.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Mo_4(C_6H_7)_4Se_4]$
M_r	1016.09
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	296
a, b, c (Å)	21.1820 (4), 8.42496 (16), 16.4482 (3)
β (°)	120.6613 (7)
V (Å³)	2524.93 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	7.72
Crystal size (mm)	$0.10 \times 0.10 \times 0.10$
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.201, 0.462
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	11868, 2878, 2617
R_{int}	0.040
$(\sin \theta/\lambda)_{max}$ (Å⁻¹)	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.021, 0.051, 1.07
No. of reflections	2878
No. of parameters	147
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	0.49, −0.79

Computer programs: RAPID AUTO (Rigaku, 2006), *SIR97* (Altomare *et al.*, 1999), *SHELXL2018/3* (Sheldrick, 2015) and *CrystalStructure* (Rigaku, 2010).

Refinement

Crystal data, date collection and structure refinement details are summarized in Table 1.

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full crystallographic data

Tetra-μ_3-selenido-1:2:3κ^3Se;1:2:4κ^3Se;1:3:4κ^3Se;2:3:4κ^3Se-tetrakis[(η^5-methyl-cyclopentadienyl)molybdenum(III)](6 *Mo—Mo*)

Akito Ouchi, Tsugiko Takase and Shinji Inomata

Tetra-μ_3-selenido-1:2:3κ^3Se;1:2:4κ^3Se;1:3:4κ^3Se;2:3:4κ^3Se-tetrakis[(η^5-methylcyclopentadienyl)molybdenum(III)] (6 *Mo—Mo*)

Crystal data

[Mo$_4$(C$_6$H$_7$)$_4$Se$_4$]
$M_r = 1016.09$
Monoclinic, $C2/c$
$a = 21.1820\ (4)$ Å
$b = 8.42496\ (16)$ Å
$c = 16.4482\ (3)$ Å
$\beta = 120.6613\ (7)°$
$V = 2524.93\ (9)$ Å^3
$Z = 4$

$F(000) = 1904.00$
$D_x = 2.673$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 10275 reflections
$\theta = 3.2–27.5°$
$\mu = 7.72$ mm^{-1}
$T = 296$ K
Platelet, brown
$0.10 \times 0.10 \times 0.10$ mm

Data collection

Rigaku R-AXIS RAPID
    diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan
    (ABSCOR; Rigaku, 1995)
$T_{min} = 0.201$, $T_{max} = 0.462$
11868 measured reflections

2878 independent reflections
2617 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -24 \rightarrow 27$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.051$
$S = 1.07$
2878 reflections
147 parameters
0 restraints
Primary atom site location: structure-invariant
    direct methods

Secondary atom site location: difference Fourier
    map
Hydrogen site location: inferred from
    neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0168P)^2 + 4.2366P]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}

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 was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

All hydrogen atoms were placed at calculated positions (C—H = 0.96–0.98 Å) and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

	x	y	z	$U_{iso}*/U_{eq}$
Mo1	−0.05709 (2)	0.36774 (3)	0.77761 (2)	0.01956 (7)
Mo2	0.05898 (2)	0.11729 (3)	0.85272 (2)	0.02062 (7)
Se1	−0.07420 (2)	0.07974 (3)	0.78522 (2)	0.02368 (8)
Se2	0.07609 (2)	0.40514 (3)	0.88225 (2)	0.02324 (8)
C1	−0.16873 (18)	0.4032 (4)	0.7760 (2)	0.0334 (7)
C2	−0.16199 (18)	0.5254 (4)	0.7228 (2)	0.0317 (7)
H1	−0.197372	0.548621	0.656343	0.038*
C3	−0.1002 (2)	0.6197 (4)	0.7834 (2)	0.0344 (7)
H2	−0.086145	0.719615	0.766422	0.041*
C4	−0.0688 (2)	0.5553 (4)	0.8753 (2)	0.0350 (7)
H3	−0.028235	0.601956	0.932877	0.042*
C5	−0.10922 (19)	0.4220 (4)	0.8715 (2)	0.0332 (7)
H4	−0.101723	0.359419	0.925903	0.040*
C6	0.0722 (2)	−0.0631 (4)	0.9693 (2)	0.0380 (8)
H5	0.032142	−0.108311	0.975354	0.046*
C7	0.1045 (2)	−0.1336 (4)	0.9208 (2)	0.0362 (8)
H6	0.090569	−0.235528	0.887498	0.043*
C8	0.16702 (18)	−0.0398 (4)	0.9400 (2)	0.0335 (7)
C9	0.1704 (2)	0.0874 (4)	0.9965 (2)	0.0381 (8)
H7	0.209754	0.166436	1.024598	0.046*
C10	0.1123 (2)	0.0738 (4)	1.0150 (2)	0.0401 (9)
H8	0.105439	0.139947	1.058922	0.048*
C11	−0.2285 (2)	0.2840 (5)	0.7442 (3)	0.0524 (10)
H9	−0.213781	0.202041	0.791047	0.063*
H10	−0.238348	0.238212	0.685470	0.063*
H11	−0.272079	0.334778	0.735713	0.063*
C12	0.2244 (2)	−0.0779 (5)	0.9148 (3)	0.0509 (10)
H12	0.250562	0.017026	0.917858	0.061*
H13	0.201080	−0.120411	0.851841	0.061*
H14	0.258069	−0.154750	0.958472	0.061*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.02236 (13)	0.01507 (12)	0.01911 (12)	0.00142 (9)	0.00902 (10)	−0.00024 (9)

Mo2	0.02366 (13)	0.01577 (12)	0.01921 (12)	0.00191 (9)	0.00860 (10)	0.00260 (9)
Se1	0.02711 (16)	0.01821 (15)	0.02549 (15)	−0.00290 (11)	0.01325 (12)	0.00020 (11)
Se2	0.02603 (16)	0.01916 (14)	0.01959 (14)	−0.00302 (11)	0.00805 (12)	−0.00285 (11)
C1	0.0301 (17)	0.0359 (18)	0.0375 (17)	0.0050 (14)	0.0196 (14)	−0.0026 (14)
C2	0.0305 (17)	0.0322 (17)	0.0314 (16)	0.0127 (14)	0.0151 (13)	0.0036 (14)
C3	0.042 (2)	0.0175 (14)	0.0447 (19)	0.0097 (14)	0.0232 (16)	0.0006 (14)
C4	0.0388 (19)	0.0307 (17)	0.0322 (16)	0.0051 (14)	0.0157 (14)	−0.0109 (14)
C5	0.0404 (19)	0.0358 (18)	0.0283 (15)	0.0116 (15)	0.0210 (14)	0.0031 (14)
C6	0.044 (2)	0.0360 (19)	0.0345 (17)	0.0073 (15)	0.0200 (15)	0.0200 (15)
C7	0.046 (2)	0.0199 (15)	0.0370 (17)	0.0100 (14)	0.0169 (16)	0.0127 (13)
C8	0.0306 (17)	0.0340 (18)	0.0287 (15)	0.0130 (14)	0.0099 (13)	0.0145 (14)
C9	0.0344 (19)	0.0376 (19)	0.0261 (15)	0.0056 (15)	0.0036 (14)	0.0067 (14)
C10	0.051 (2)	0.041 (2)	0.0208 (14)	0.0139 (17)	0.0122 (15)	0.0095 (14)
C11	0.039 (2)	0.055 (2)	0.068 (3)	−0.0036 (19)	0.031 (2)	−0.006 (2)
C12	0.046 (2)	0.052 (2)	0.052 (2)	0.0155 (19)	0.0230 (19)	0.0129 (19)

Geometric parameters (Å, º)

Mo1—C3	2.332 (3)	C2—C3	1.416 (5)
Mo1—C2	2.339 (3)	C2—H1	0.9800
Mo1—C4	2.355 (3)	C3—C4	1.413 (5)
Mo1—C5	2.356 (3)	C3—H2	0.9800
Mo1—C1	2.370 (3)	C4—C5	1.394 (5)
Mo1—Se2	2.4633 (4)	C4—H3	0.9800
Mo1—Se1	2.4659 (4)	C5—H4	0.9800
Mo1—Se2[i]	2.4689 (3)	C6—C10	1.402 (5)
Mo1—Mo1[i]	2.9857 (5)	C6—C7	1.419 (5)
Mo1—Mo2	2.9875 (3)	C6—H5	0.9800
Mo1—Mo2[i]	2.9935 (3)	C7—C8	1.432 (5)
Mo2—C10	2.337 (3)	C7—H6	0.9800
Mo2—C6	2.350 (3)	C8—C9	1.396 (5)
Mo2—C9	2.352 (3)	C8—C12	1.506 (5)
Mo2—C7	2.356 (3)	C9—C10	1.414 (5)
Mo2—C8	2.387 (3)	C9—H7	0.9800
Mo2—Se2	2.4635 (4)	C10—H8	0.9800
Mo2—Se1	2.4691 (4)	C11—H9	0.9600
Mo2—Se1[i]	2.4692 (4)	C11—H10	0.9600
Mo2—Mo2[i]	3.0083 (5)	C11—H11	0.9600
C1—C2	1.404 (5)	C12—H12	0.9600
C1—C5	1.435 (5)	C12—H13	0.9600
C1—C11	1.487 (5)	C12—H14	0.9600
C3—Mo1—C2	35.30 (12)	C7—Mo2—Mo1[i]	145.65 (9)
C3—Mo1—C4	35.09 (12)	C8—Mo2—Mo1[i]	118.70 (8)
C2—Mo1—C4	58.11 (11)	Se2—Mo2—Mo1[i]	52.718 (9)
C3—Mo1—C5	58.16 (12)	Se1—Mo2—Mo1[i]	99.982 (11)
C2—Mo1—C5	58.09 (11)	Se1[i]—Mo2—Mo1[i]	52.606 (9)
C4—Mo1—C5	34.41 (12)	Mo1—Mo2—Mo1[i]	59.894 (10)

C3—Mo1—C1	58.43 (12)	C10—Mo2—Mo2i	157.50 (10)
C2—Mo1—C1	34.69 (12)	C6—Mo2—Mo2i	127.01 (9)
C4—Mo1—C1	58.08 (12)	C9—Mo2—Mo2i	164.17 (9)
C5—Mo1—C1	35.36 (11)	C7—Mo2—Mo2i	115.98 (9)
C3—Mo1—Se2	100.84 (9)	C8—Mo2—Mo2i	131.90 (8)
C2—Mo1—Se2	136.14 (9)	Se2—Mo2—Mo2i	100.132 (8)
C4—Mo1—Se2	85.36 (9)	Se1—Mo2—Mo2i	52.472 (10)
C5—Mo1—Se2	105.65 (9)	Se1i—Mo2—Mo2i	52.471 (10)
C1—Mo1—Se2	140.55 (8)	Mo1—Mo2—Mo2i	59.902 (8)
C3—Mo1—Se1	145.37 (9)	Mo1i—Mo2—Mo2i	59.705 (8)
C2—Mo1—Se1	116.29 (9)	Mo1—Se1—Mo2	74.510 (12)
C4—Mo1—Se1	123.79 (9)	Mo1—Se1—Mo2i	74.684 (11)
C5—Mo1—Se1	91.58 (9)	Mo2—Se1—Mo2i	75.060 (13)
C1—Mo1—Se1	87.30 (8)	Mo1—Se2—Mo2	74.656 (12)
Se2—Mo1—Se1	103.651 (13)	Mo1—Se2—Mo1i	74.507 (12)
C3—Mo1—Se2i	94.16 (9)	Mo2—Se2—Mo1i	74.730 (11)
C2—Mo1—Se2i	84.87 (8)	C2—C1—C5	106.8 (3)
C4—Mo1—Se2i	128.63 (9)	C2—C1—C11	128.0 (3)
C5—Mo1—Se2i	142.82 (8)	C5—C1—C11	125.1 (3)
C1—Mo1—Se2i	110.62 (8)	C2—C1—Mo1	71.44 (19)
Se2—Mo1—Se2i	103.560 (13)	C5—C1—Mo1	71.77 (18)
Se1—Mo1—Se2i	103.372 (13)	C11—C1—Mo1	125.8 (2)
C3—Mo1—Mo1i	114.04 (9)	C1—C2—C3	108.9 (3)
C2—Mo1—Mo1i	129.84 (8)	C1—C2—Mo1	73.87 (18)
C4—Mo1—Mo1i	126.24 (9)	C3—C2—Mo1	72.07 (17)
C5—Mo1—Mo1i	157.28 (9)	C1—C2—H1	125.4
C1—Mo1—Mo1i	162.73 (8)	C3—C2—H1	125.4
Se2—Mo1—Mo1i	52.834 (10)	Mo1—C2—H1	125.4
Se1—Mo1—Mo1i	100.268 (9)	C4—C3—C2	107.4 (3)
Se2i—Mo1—Mo1i	52.659 (10)	C4—C3—Mo1	73.37 (18)
C3—Mo1—Mo2	152.01 (9)	C2—C3—Mo1	72.64 (17)
C2—Mo1—Mo2	168.55 (9)	C4—C3—H2	126.0
C4—Mo1—Mo2	122.87 (8)	C2—C3—H2	126.0
C5—Mo1—Mo2	115.34 (8)	Mo1—C3—H2	126.0
C1—Mo1—Mo2	134.39 (8)	C5—C4—C3	108.5 (3)
Se2—Mo1—Mo2	52.676 (10)	C5—C4—Mo1	72.81 (18)
Se1—Mo1—Mo2	52.794 (10)	C3—C4—Mo1	71.54 (17)
Se2i—Mo1—Mo2	100.565 (11)	C5—C4—H3	125.6
Mo1i—Mo1—Mo2	60.153 (8)	C3—C4—H3	125.6
C3—Mo1—Mo2i	143.92 (9)	Mo1—C4—H3	125.6
C2—Mo1—Mo2i	117.47 (8)	C4—C5—C1	108.4 (3)
C4—Mo1—Mo2i	173.63 (9)	C4—C5—Mo1	72.78 (18)
C5—Mo1—Mo2i	140.04 (9)	C1—C5—Mo1	72.87 (17)
C1—Mo1—Mo2i	115.58 (8)	C4—C5—H4	125.6
Se2—Mo1—Mo2i	100.539 (11)	C1—C5—H4	125.6
Se1—Mo1—Mo2i	52.709 (9)	Mo1—C5—H4	125.6
Se2i—Mo1—Mo2i	52.551 (9)	C10—C6—C7	108.1 (3)
Mo1i—Mo1—Mo2i	59.954 (8)	C10—C6—Mo2	72.11 (18)

Mo2—Mo1—Mo2[i]	60.394 (10)	C7—C6—Mo2	72.68 (17)
C10—Mo2—C6	34.82 (13)	C10—C6—H5	125.8
C10—Mo2—C9	35.10 (13)	C7—C6—H5	125.8
C6—Mo2—C9	57.92 (13)	Mo2—C6—H5	125.8
C10—Mo2—C7	58.26 (13)	C6—C7—C8	107.6 (3)
C6—Mo2—C7	35.11 (12)	C6—C7—Mo2	72.22 (18)
C9—Mo2—C7	57.88 (13)	C8—C7—Mo2	73.65 (18)
C10—Mo2—C8	57.94 (12)	C6—C7—H6	126.0
C6—Mo2—C8	58.10 (12)	C8—C7—H6	126.0
C9—Mo2—C8	34.26 (12)	Mo2—C7—H6	126.0
C7—Mo2—C8	35.14 (12)	C9—C8—C7	107.3 (3)
C10—Mo2—Se2	89.56 (9)	C9—C8—C12	125.0 (3)
C6—Mo2—Se2	122.11 (9)	C7—C8—C12	127.4 (3)
C9—Mo2—Se2	86.33 (9)	C9—C8—Mo2	71.47 (18)
C7—Mo2—Se2	143.71 (9)	C7—C8—Mo2	71.21 (18)
C8—Mo2—Se2	115.33 (9)	C12—C8—Mo2	127.8 (2)
C10—Mo2—Se1	105.64 (10)	C8—C9—C10	109.1 (3)
C6—Mo2—Se1	85.26 (9)	C8—C9—Mo2	74.27 (18)
C9—Mo2—Se1	140.23 (9)	C10—C9—Mo2	71.88 (18)
C7—Mo2—Se1	101.27 (9)	C8—C9—H7	125.3
C8—Mo2—Se1	136.41 (9)	C10—C9—H7	125.3
Se2—Mo2—Se1	103.549 (13)	Mo2—C9—H7	125.3
C10—Mo2—Se1[i]	144.67 (10)	C6—C10—C9	107.9 (3)
C6—Mo2—Se1[i]	130.55 (9)	C6—C10—Mo2	73.08 (18)
C9—Mo2—Se1[i]	112.09 (9)	C9—C10—Mo2	73.01 (18)
C7—Mo2—Se1[i]	96.22 (9)	C6—C10—H8	125.8
C8—Mo2—Se1[i]	86.98 (8)	C9—C10—H8	125.8
Se2—Mo2—Se1[i]	103.434 (13)	Mo2—C10—H8	125.8
Se1—Mo2—Se1[i]	103.004 (13)	C1—C11—H9	109.5
C10—Mo2—Mo1	113.56 (9)	C1—C11—H10	109.5
C6—Mo2—Mo1	121.66 (9)	H9—C11—H10	109.5
C9—Mo2—Mo1	133.12 (9)	C1—C11—H11	109.5
C7—Mo2—Mo1	151.79 (9)	H9—C11—H11	109.5
C8—Mo2—Mo1	167.07 (9)	H10—C11—H11	109.5
Se2—Mo2—Mo1	52.668 (10)	C8—C12—H12	109.5
Se1—Mo2—Mo1	52.696 (9)	C8—C12—H13	109.5
Se1[i]—Mo2—Mo1	100.141 (11)	H12—C12—H13	109.5
C10—Mo2—Mo1[i]	138.65 (10)	C8—C12—H14	109.5
C6—Mo2—Mo1[i]	173.27 (10)	H12—C12—H14	109.5
C9—Mo2—Mo1[i]	115.84 (9)	H13—C12—H14	109.5
C5—C1—C2—C3	−0.5 (4)	C10—C6—C7—C8	1.8 (4)
C11—C1—C2—C3	174.6 (3)	Mo2—C6—C7—C8	65.7 (2)
Mo1—C1—C2—C3	−64.0 (2)	C10—C6—C7—Mo2	−63.8 (2)
C5—C1—C2—Mo1	63.5 (2)	C6—C7—C8—C9	−2.0 (3)
C11—C1—C2—Mo1	−121.4 (4)	Mo2—C7—C8—C9	62.8 (2)
C1—C2—C3—C4	−0.5 (4)	C6—C7—C8—C12	171.5 (3)
Mo1—C2—C3—C4	−65.7 (2)	Mo2—C7—C8—C12	−123.7 (3)

C1—C2—C3—Mo1	65.2 (2)	C6—C7—C8—Mo2	−64.7 (2)
C2—C3—C4—C5	1.3 (4)	C7—C8—C9—C10	1.3 (3)
Mo1—C3—C4—C5	−63.9 (2)	C12—C8—C9—C10	−172.4 (3)
C2—C3—C4—Mo1	65.2 (2)	Mo2—C8—C9—C10	63.9 (2)
C3—C4—C5—C1	−1.6 (4)	C7—C8—C9—Mo2	−62.6 (2)
Mo1—C4—C5—C1	−64.7 (2)	C12—C8—C9—Mo2	123.7 (3)
C3—C4—C5—Mo1	63.0 (2)	C7—C6—C10—C9	−1.0 (4)
C2—C1—C5—C4	1.3 (4)	Mo2—C6—C10—C9	−65.2 (2)
C11—C1—C5—C4	−173.9 (3)	C7—C6—C10—Mo2	64.2 (2)
Mo1—C1—C5—C4	64.6 (2)	C8—C9—C10—C6	−0.2 (4)
C2—C1—C5—Mo1	−63.3 (2)	Mo2—C9—C10—C6	65.3 (2)
C11—C1—C5—Mo1	121.4 (3)	C8—C9—C10—Mo2	−65.5 (2)

Symmetry code: (i) $-x, y, -z+3/2$.