

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.026$

$S = 1.74$

1121 reflections

31 parameters

$\Delta\rho_{\max} = 2.64 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -1.57 \text{ e } \text{Å}^{-3}$

The Chevrel phase HgMo_6S_8

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Received 16 March 2009; accepted 2 April 2009

Key indicators: single-crystal X-ray study; $T = 293 \text{ K}$; mean $\sigma(\text{Mo}-\text{S}) = 0.001 \text{ Å}$; disorder in main residue; R factor = 0.025; wR factor = 0.026; data-to-parameter ratio = 36.2.

The crystal structure of HgMo_6S_8 , mercury(II) hexamolybdenum octasulfide, is based on $(\text{Mo}_6\text{S}_8)\text{S}_6$ cluster units ($\bar{3}$ symmetry) interconnected through interunit Mo—S bonds. The Hg^{2+} cations occupy large voids between the different cluster units and are covalently bonded to two S atoms. The Hg atoms and one S atom lie on sites with crystallographic $\bar{3}$ and 3 symmetry, respectively. Refinement of the occupancy factor of the Hg atom led to the composition $\text{Hg}_{0.973(3)}\text{Mo}_6\text{S}_8$.

Related literature

For isotypic structures, see: Chevrel & Sergent (1982). For a previous report on the title compound as a polycrystalline material, see: Tarascon *et al.* (1983). For crystallographic background, see: Becker & Coppens (1974); Johnson & Levy (1974).

Experimental

Crystal data

$\text{Hg}_{0.973}\text{Mo}_6\text{S}_8$	$Z = 3$
$M_r = 1027.3$	Mo $K\alpha$ radiation
Trigonal, $R\bar{3}$	$\mu = 21.62 \text{ mm}^{-1}$
$a = 9.4319(3) \text{ Å}$	$T = 293 \text{ K}$
$c = 10.7028(3) \text{ Å}$	$0.08 \times 0.07 \times 0.06 \text{ mm}$
$V = 824.57(4) \text{ Å}^3$	

Data collection

Nonius KappaCCD diffractometer	5784 measured reflections
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	1121 independent reflections
$T_{\min} = 0.298$, $T_{\max} = 0.384$	1069 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.044$

Table 1

Selected bond lengths (Å).

Hg1—S1	2.3914 (8)	Mo1—S2	2.4236 (6)
Mo1—Mo1 ⁱ	2.7184 (3)	Mo1—S2 ⁱⁱⁱ	2.4896 (8)
Mo1—Mo1 ⁱⁱ	2.7515 (3)	Mo1—S2 ⁱⁱ	2.4933 (6)
Mo1—S1	2.4108 (7)	Mo1—S2 ^{iv}	2.4340 (8)

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

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: *JANA2000* (Petříček & Dušek, 2000); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *JANA2000*.

Intensity data were collected on the Nonius KappaCCD X-ray diffractometer system of 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: WM2226).

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supporting information

Acta Cryst. (2009). E65, i34 [doi:10.1107/S1600536809012495]

The Chevrel phase HgMo_6S_8

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S1. Comment

The superconducting compound HgMo_6S_8 was first synthesized as a powder sample by Tarascon *et al.* (1983), but no details were given on its crystal structure. In the present study, we present the crystal structure refinement of HgMo_6S_8 that has been determined from single-crystal X-ray diffraction data. The title compound is isostructural with the hexagonal Chevrel phases $M\text{Mo}_6\text{X}_8$ where M is a large cation ($M = \text{alkali metal, alkaline earth, lanthanide, actinide etc.}; X = \text{S, Se, Te}$) [see, for instance, Chevrel & Sergent (1982)]. As a consequence its crystal structure consists of octahedral Mo_6 clusters surrounded by fourteen sulfur atoms with eight of them forming a distorted cube (i -type ligands) and the remaining six capping the faces of the S_8 cube (a -type ligands). In the structure of HgMo_6S_8 , a part of the chalcogen atoms of the $\text{Mo}_6\text{S}_8^i\text{S}_6^a$ unit are shared according to the formula $\text{Mo}_6\text{S}_2^i\text{S}_4^a$ to form the three-dimensional Mo—S network. The Mo_6S_8 cluster unit is centered at Wyckoff position $6b$ ($\bar{3}$ symmetry). The Mo—Mo distances within the Mo_6 clusters are 2.7184 (3) Å for the intra-triangle distances (distances within the Mo_3 triangles formed by the Mo atoms related through the threefold axis) and 2.7515 (3) Å for the inter-triangle distances. Each Mo atom is surrounded by five S atoms (4 S1 and 1 S2) forming a distorted square-based pyramid. The apex of the pyramid is shared with an adjacent unit and thus ensures the three-dimensional cohesion. Consequently, each Mo_6S_8 unit is interconnected to 6 Mo_6S_8 units to form the Mo—S framework. It results from this arrangement that the shortest intercluster Mo1—Mo1 distances between the Mo_6 clusters is 3.2934 (3) Å, indicating only weak metal-metal interaction. The Hg^{2+} cations reside in the large eight-coordinate voids formed by the chalcogen atoms from eight different Mo_6S_8 units. They are covalently bonded to two S2 atoms at a distance of 2.3914 (8) Å.

HgMo_6S_8 was found to be superconducting at 8 K from DC-susceptibility measurements on a batch of single crystals.

S2. Experimental

HgMo_6S_8 was obtained in three steps involving, first, the syntheses of single-crystal of InMo_6S_8 by solid state reaction, then the preparation of the binary compound Mo_6S_8 by 'chimie douce' methods and, finally, the synthesis of the title compound by inserting mercury into the Mo_6S_8 host structure at low temperatures. Single crystals of InMo_6S_8 were obtained from a stoichiometric mixture of In_2S_3 , MoS_2 and Mo. 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 six hours, then cooled at 100 K/h down to 1273 K and finally furnace cooled. Mo_6S_8 was obtained by oxidation of single-crystals of InMo_6S_8 by iodine in a glass tube sealed under vacuum. The end of the tube containing the crystals of the In compound and an excess of iodine was placed in a furnace with about 3 cm of the other end sticking out of the furnace, at about room temperature. The furnace was then heated at 523 K for 96 h. At the end of the reaction, crystals of InI_3 and I_2 were obtained at the cooler end of the tube. Finally, HgMo_6S_8 was prepared by diffusion of mercury into crystals of Mo_6S_8 in a silica glass tube sealed under vacuum at 673 K during 96 h.

S3. Refinement

The structure was refined using an anisotropic approximation and converged at a reliability factor $R(F) = 0.034$. Analyses of the difference Fourier maps revealed positive and negative residual peaks around the Hg atom. Fourth-order tensors in the Gram-Charlier expansion (Johnson & Levy, 1974) of the mercury displacement factor were used to describe the electron density around this site. The resulting R value dropped to 0.025 for only five additional parameters. Refinement of the occupancy factor of the Hg atom led to the final composition $\text{Hg}_{0.973(3)}\text{Mo}_6\text{S}_8$.

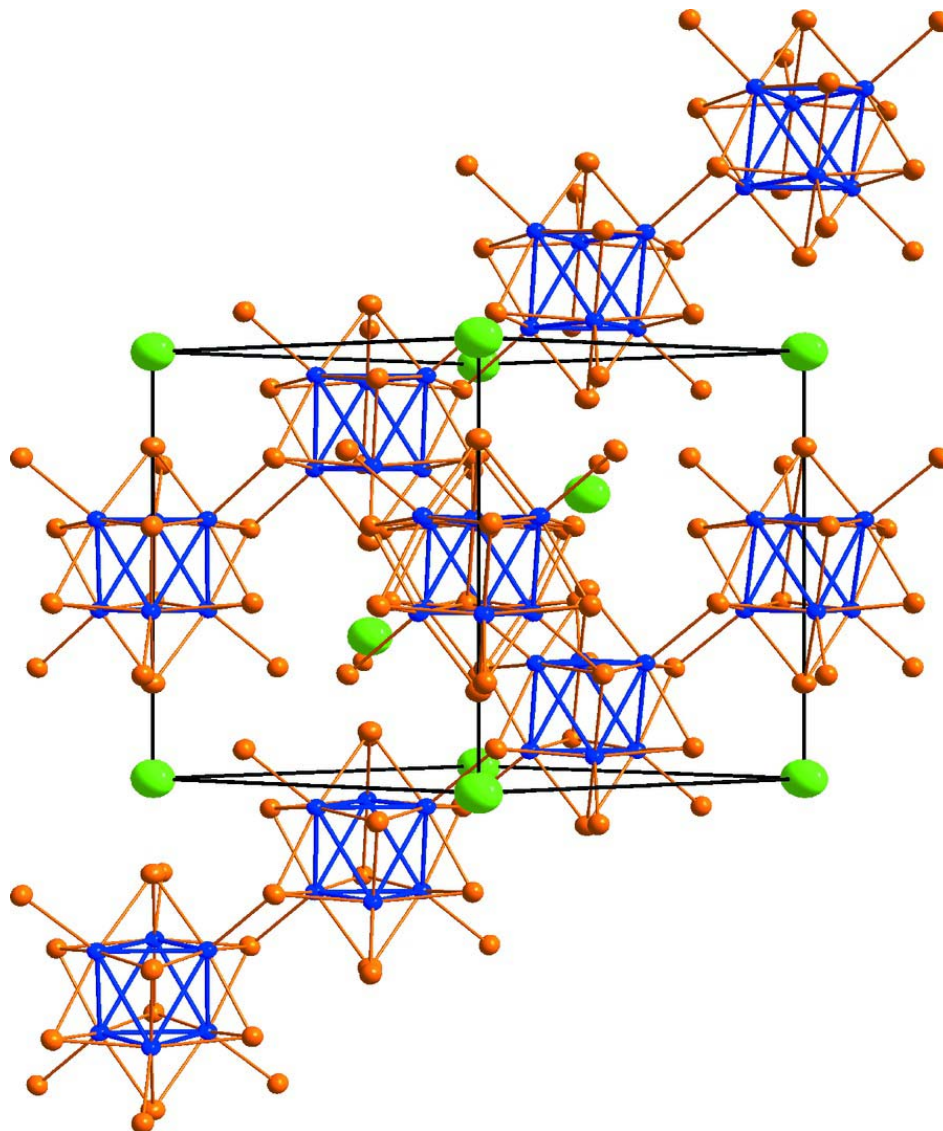
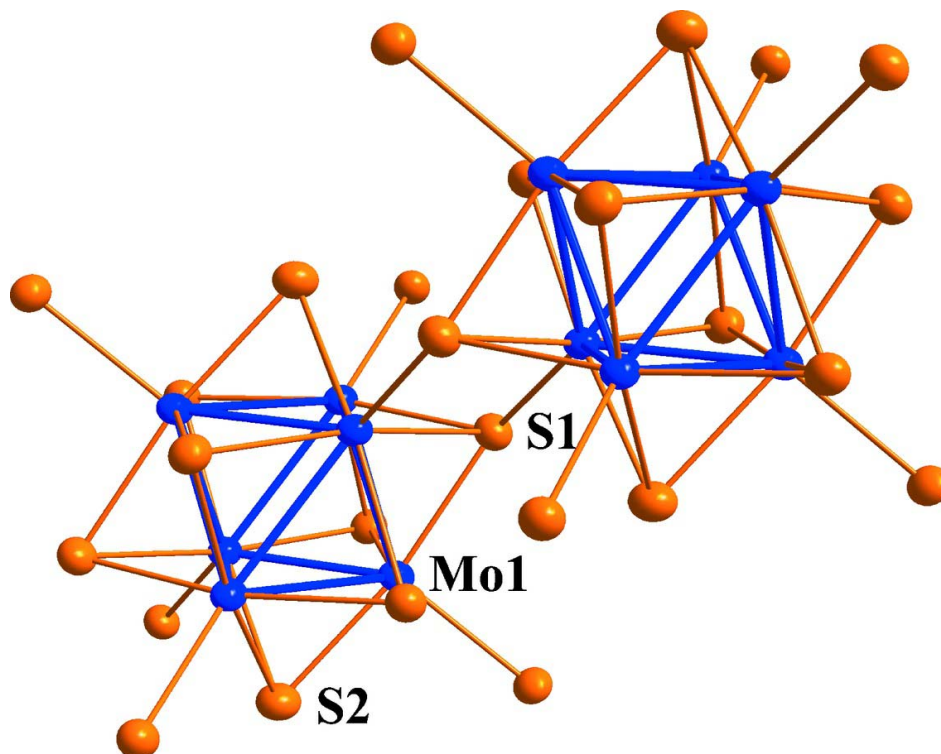


Figure 1

View of HgMo_6S_8 along $[110]$.

**Figure 2**

Plot showing the atom-numbering scheme and the interunit linkage of the $(\text{Mo}_6\text{S}_8)\text{S}_6$ cluster units. Displacement ellipsoids are drawn at the 97% probability level.

(I)*Crystal data* $\text{Hg}_{0.973}\text{Mo}_6\text{S}_8$ $M_r = 1027.3$ Trigonal, $R\bar{3}$

Hall symbol: -R 3

 $a = 9.4319 (3) \text{ \AA}$ $c = 10.7028 (3) \text{ \AA}$ $V = 824.57 (4) \text{ \AA}^3$ $Z = 3$ $F(000) = 1374$ *Data collection*Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

Horizontally mounted graphite crystal
monochromatorDetector resolution: 9 pixels mm^{-1} ω - and φ -scansAbsorption correction: analytical
(de Meulenaer & Tompa, 1965) $D_x = 6.204 (1) \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 7043 reflections

 $\theta = 2.0\text{--}42.1^\circ$ $\mu = 21.62 \text{ mm}^{-1}$ $T = 293 \text{ K}$

Truncated cube, black

 $0.08 \times 0.07 \times 0.06 \text{ mm}$ $T_{\min} = 0.298, T_{\max} = 0.384$

5784 measured reflections

1121 independent reflections

1069 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.044$ $\theta_{\max} = 39.8^\circ, \theta_{\min} = 3.1^\circ$ $h = -16 \rightarrow 16$ $k = -16 \rightarrow 16$ $l = -13 \rightarrow 19$

Refinement

Refinement on F
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.026$
 $S = 1.74$
 1121 reflections
 31 parameters

Weighting scheme based on measured s.u.'s $w = 1/\sigma^2(F)$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 2.64 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.57 \text{ e } \text{\AA}^{-3}$
 Extinction correction: B-C type 1 Lorentzian isotropic (Becker & Coppens, 1974)
 Extinction coefficient: 0.020681

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Hg1	0	0	0	0.0339 (4)	0.973 (3)
Mo1	-0.01555 (2)	-0.17363 (2)	-0.394419 (15)	0.00748 (7)	
S1	0	0	-0.22344 (8)	0.0113 (2)	
S2	-0.03460 (6)	-0.31591 (7)	-0.58775 (4)	0.00933 (17)	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0384 (4)	0.0384 (4)	0.0249 (6)	0.0192 (2)	0	0
Mo1	0.00780 (9)	0.00831 (9)	0.00617 (10)	0.00391 (6)	0.00003 (5)	-0.00036 (5)
S1	0.0126 (2)	0.0126 (2)	0.0088 (3)	0.00628 (12)	0	0
S2	0.0097 (2)	0.0096 (2)	0.0087 (2)	0.00476 (17)	0.00067 (15)	-0.00032 (15)

Geometric parameters (\AA , $^\circ$)

Hg1—S1	2.3914 (8)	Mo1—Mo1 ^{ix}	2.7184 (3)
Hg1—S1 ⁱ	2.3914 (8)	Mo1—Mo1 ^x	2.7515 (3)
Hg1—S2 ⁱⁱ	3.2056 (4)	Mo1—Mo1 ^{xi}	2.7184 (4)
Hg1—S2 ⁱⁱⁱ	3.2056 (4)	Mo1—Mo1 ^{xii}	2.7515 (2)
Hg1—S2 ^{iv}	3.2056 (7)	Mo1—S1	2.4108 (7)
Hg1—S2 ^v	3.2056 (7)	Mo1—S2	2.4236 (6)
Hg1—S2 ^{vi}	3.2056 (8)	Mo1—S2 ^{xiii}	2.4896 (8)
Hg1—S2 ^{vii}	3.2056 (8)	Mo1—S2 ^x	2.4933 (6)
Mo1—Mo1 ^{viii}	3.8679 (3)	Mo1—S2 ^{xii}	2.4340 (8)
Mo1—Mo1 ⁱⁱⁱ	3.2131 (2)		
S1—Hg1—S1 ⁱ	180	Mo1 ^x —Mo1—Mo1 ⁱⁱⁱ	97.693 (7)
S1—Hg1—S2 ⁱⁱ	105.278 (8)	Mo1 ^x —Mo1—Mo1 ^{ix}	90
S1—Hg1—S2 ⁱⁱⁱ	74.722 (8)	Mo1 ^x —Mo1—Mo1 ^{xi}	60.398 (8)
S1—Hg1—S2 ^{iv}	105.278 (9)	Mo1 ^x —Mo1—Mo1 ^{xii}	59.205 (7)
S1—Hg1—S2 ^v	74.722 (9)	Mo1 ^x —Mo1—S1	115.964 (15)
S1—Hg1—S2 ^{vi}	105.278 (9)	Mo1 ^x —Mo1—S2	55.677 (18)
S1—Hg1—S2 ^{vii}	74.722 (9)	Mo1 ^x —Mo1—S2 ^{xiii}	138.626 (14)
S1 ⁱ —Hg1—S1	180	Mo1 ^x —Mo1—S2 ^x	54.776 (13)
S1 ⁱ —Hg1—S2 ⁱⁱ	74.722 (8)	Mo1 ^x —Mo1—S2 ^{xii}	114.515 (14)
S1 ⁱ —Hg1—S2 ⁱⁱⁱ	105.278 (8)	Mo1 ^{xi} —Mo1—Mo1 ⁱⁱⁱ	96.739 (8)

S1 ⁱ —Hg1—S2 ^{iv}	74.722 (9)	Mo1 ^{xi} —Mo1—Mo1 ^{ix}	60.000 (8)
S1 ⁱ —Hg1—S2 ^v	105.278 (9)	Mo1 ^{xi} —Mo1—Mo1 ^x	60.398 (8)
S1 ⁱ —Hg1—S2 ^{vi}	74.722 (9)	Mo1 ^{xi} —Mo1—Mo1 ^{xii}	90
S1 ⁱ —Hg1—S2 ^{vii}	105.278 (9)	Mo1 ^{xi} —Mo1—S1	55.682 (12)
S2 ⁱⁱ —Hg1—S2 ⁱⁱⁱ	180	Mo1 ^{xi} —Mo1—S2	116.065 (18)
S2 ⁱⁱ —Hg1—S2 ^{iv}	113.319 (18)	Mo1 ^{xi} —Mo1—S2 ^{xiii}	135.971 (18)
S2 ⁱⁱ —Hg1—S2 ^v	66.681 (18)	Mo1 ^{xi} —Mo1—S2 ^x	55.48 (2)
S2 ⁱⁱ —Hg1—S2 ^{vi}	113.319 (17)	Mo1 ^{xi} —Mo1—S2 ^{xii}	117.362 (19)
S2 ⁱⁱ —Hg1—S2 ^{vii}	66.681 (17)	Mo1 ^{xii} —Mo1—Mo1 ⁱⁱⁱ	148.317 (7)
S2 ⁱⁱⁱ —Hg1—S2 ⁱⁱ	180	Mo1 ^{xii} —Mo1—Mo1 ^{ix}	60.398 (6)
S2 ⁱⁱⁱ —Hg1—S2 ^{iv}	66.681 (18)	Mo1 ^{xii} —Mo1—Mo1 ^x	59.205 (7)
S2 ⁱⁱⁱ —Hg1—S2 ^v	113.319 (18)	Mo1 ^{xii} —Mo1—Mo1 ^{xi}	90
S2 ⁱⁱⁱ —Hg1—S2 ^{vi}	66.681 (17)	Mo1 ^{xii} —Mo1—S1	115.964 (13)
S2 ⁱⁱⁱ —Hg1—S2 ^{vii}	113.319 (17)	Mo1 ^{xii} —Mo1—S2	57.184 (12)
S2 ^{iv} —Hg1—S2 ⁱⁱ	113.319 (18)	Mo1 ^{xii} —Mo1—S2 ^{xiii}	133.837 (19)
S2 ^{iv} —Hg1—S2 ⁱⁱⁱ	66.681 (18)	Mo1 ^{xii} —Mo1—S2 ^x	113.894 (15)
S2 ^{iv} —Hg1—S2 ^v	180	Mo1 ^{xii} —Mo1—S2 ^{xii}	55.318 (14)
S2 ^{iv} —Hg1—S2 ^{vi}	113.319 (19)	S1—Mo1—S2	170.65 (2)
S2 ^{iv} —Hg1—S2 ^{vii}	66.681 (19)	S1—Mo1—S2 ^{xiii}	93.53 (2)
S2 ^v —Hg1—S2 ⁱⁱ	66.681 (18)	S1—Mo1—S2 ^x	90.323 (17)
S2 ^v —Hg1—S2 ⁱⁱⁱ	113.319 (18)	S1—Mo1—S2 ^{xii}	91.758 (14)
S2 ^v —Hg1—S2 ^{iv}	180	S2—Mo1—S2 ^{xiii}	95.79 (2)
S2 ^v —Hg1—S2 ^{vi}	66.681 (19)	S2—Mo1—S2 ^x	87.39 (2)
S2 ^v —Hg1—S2 ^{vii}	113.319 (19)	S2—Mo1—S2 ^{xii}	88.750 (19)
S2 ^{vi} —Hg1—S2 ⁱⁱ	113.319 (17)	S2 ^{xiii} —Mo1—S2	95.79 (2)
S2 ^{vi} —Hg1—S2 ⁱⁱⁱ	66.681 (17)	S2 ^{xiii} —Mo1—S2 ^x	99.70 (2)
S2 ^{vi} —Hg1—S2 ^{iv}	113.319 (19)	S2 ^{xiii} —Mo1—S2 ^{xii}	91.39 (2)
S2 ^{vi} —Hg1—S2 ^v	66.681 (19)	S2 ^x —Mo1—S2	87.39 (2)
S2 ^{vi} —Hg1—S2 ^{vii}	180	S2 ^x —Mo1—S2 ^{xiii}	99.70 (2)
S2 ^{vii} —Hg1—S2 ⁱⁱ	66.681 (17)	S2 ^x —Mo1—S2 ^{xii}	168.58 (2)
S2 ^{vii} —Hg1—S2 ⁱⁱⁱ	113.319 (17)	S2 ^{xii} —Mo1—S2	88.750 (19)
S2 ^{vii} —Hg1—S2 ^{iv}	66.681 (19)	S2 ^{xii} —Mo1—S2 ^{xiii}	91.39 (2)
S2 ^{vii} —Hg1—S2 ^v	113.319 (19)	S2 ^{xii} —Mo1—S2 ^x	168.58 (2)
S2 ^{vii} —Hg1—S2 ^{vi}	180	Hg1—S1—Mo1	139.382 (14)
Mo1 ^{viii} —Mo1—Mo1 ⁱⁱⁱ	133.459 (8)	Hg1—S1—Mo1 ^{ix}	139.382 (13)
Mo1 ^{viii} —Mo1—S1	85.136 (14)	Hg1—S1—Mo1 ^{xi}	139.382 (14)
Mo1 ^{viii} —Mo1—S2	85.600 (16)	Mo1—S1—Mo1 ^{ix}	68.64 (2)
Mo1 ^{viii} —Mo1—S2 ^{xiii}	176.394 (13)	Mo1—S1—Mo1 ^{xi}	68.64 (2)
Mo1 ^{viii} —Mo1—S2 ^x	83.677 (18)	Mo1 ^{ix} —S1—Mo1	68.64 (2)
Mo1 ^{viii} —Mo1—S2 ^{xii}	85.310 (16)	Mo1 ^{ix} —S1—Mo1 ^{xi}	68.64 (2)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^{viii}	133.459 (8)	Mo1 ^{xi} —S1—Mo1	68.64 (2)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^{ix}	147.479 (10)	Mo1 ^{xi} —S1—Mo1 ^{ix}	68.64 (2)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^x	97.693 (7)	Hg1 ^{xiv} —S2—Mo1	125.450 (18)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^{xi}	96.739 (8)	Hg1 ^{xiv} —S2—Mo1 ^x	98.407 (18)
Mo1 ⁱⁱⁱ —Mo1—Mo1 ^{xii}	148.317 (7)	Hg1 ^{xiv} —S2—Mo1 ^{xv}	97.225 (18)
Mo1 ⁱⁱⁱ —Mo1—S1	92.988 (11)	Hg1 ^{xiv} —S2—Mo1 ^{xii}	156.59 (2)
Mo1 ⁱⁱⁱ —Mo1—S2	92.457 (12)	Mo1—S2—Mo1 ^x	69.005 (19)
Mo1 ⁱⁱⁱ —Mo1—S2 ^{xiii}	49.898 (13)	Mo1—S2—Mo1 ^{xv}	132.74 (2)

Mo1 ⁱⁱⁱ —Mo1—S2 ^x	49.797 (18)	Mo1—S2—Mo1 ^{xii}	68.041 (15)
Mo1 ⁱⁱⁱ —Mo1—S2 ^{xii}	141.203 (18)	Mo1 ^x —S2—Mo1	69.005 (19)
Mo1 ^{ix} —Mo1—Mo1 ⁱⁱⁱ	147.479 (10)	Mo1 ^x —S2—Mo1 ^{xv}	129.09 (2)
Mo1 ^{ix} —Mo1—Mo1 ^x	90	Mo1 ^x —S2—Mo1 ^{xii}	66.955 (19)
Mo1 ^{ix} —Mo1—Mo1 ^{xi}	60.000 (8)	Mo1 ^{xv} —S2—Mo1	132.74 (2)
Mo1 ^{ix} —Mo1—Mo1 ^{xii}	60.398 (6)	Mo1 ^{xv} —S2—Mo1 ^x	129.09 (2)
Mo1 ^{ix} —Mo1—S1	55.682 (11)	Mo1 ^{xv} —S2—Mo1 ^{xii}	80.305 (15)
Mo1 ^{ix} —Mo1—S2	117.489 (13)	Mo1 ^{xii} —S2—Mo1	68.041 (15)
Mo1 ^{ix} —Mo1—S2 ^{xiii}	131.337 (14)	Mo1 ^{xii} —S2—Mo1 ^x	66.955 (19)
Mo1 ^{ix} —Mo1—S2 ^x	115.28 (2)	Mo1 ^{xii} —S2—Mo1 ^{xv}	80.305 (15)
Mo1 ^{ix} —Mo1—S2 ^{xii}	57.566 (18)		

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