

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  $\text{HgMo}_6\text{S}_8$ 

Diala Salloum, Patrick Gougeon\* and Michel Potel

Laboratoire de Chimie du Solide et Inorganique Moléculaire, URA CNRS No. 6511, Université de Rennes I, Avenue du Général Leclerc, 35042 Rennes CEDEX, France  
Correspondence e-mail: Patrick.Gougeon@univ-rennes1.fr

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.

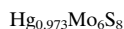
The crystal structure of  $\text{HgMo}_6\text{S}_8$ , mercury(II) hexamolybdenum octasulfide, is based on  $(\text{Mo}_6\text{S}_8)\text{S}_6$  cluster units ( $\bar{3}$  symmetry) interconnected through interunit Mo—S bonds. The  $\text{Hg}^{2+}$  cations occupy large voids between the different cluster 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



$M_r = 1027.3$

Trigonal,  $R\bar{3}$ 

$a = 9.4319(3) \text{ Å}$

$c = 10.7028(3) \text{ Å}$

$V = 824.57(4) \text{ Å}^3$

$Z = 3$

Mo  $K\alpha$  radiation

$\mu = 21.62 \text{ mm}^{-1}$

$T = 293 \text{ K}$

$0.08 \times 0.07 \times 0.06 \text{ mm}$

## Data collection

Nonius KappaCCD diffractometer

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

$T_{\min} = 0.298, T_{\max} = 0.384$

5784 measured reflections

1121 independent reflections

1069 reflections with  $I > 2\sigma(I)$ 

$R_{\text{int}} = 0.044$

Table 1

Selected bond lengths (Å).

Hg1—S1	2.3914 (8)	Mo1—S2	2.4236 (6)
Mo1—Mo1 <sup>i</sup>	2.7184 (3)	Mo1—S2 <sup>iii</sup>	2.4896 (8)
Mo1—Mo1 <sup>ii</sup>	2.7515 (3)	Mo1—S2 <sup>ii</sup>	2.4933 (6)
Mo1—S1	2.4108 (7)	Mo1—S2 <sup>iv</sup>	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](http://www.cdifx.univ-rennes1.fr)).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2226).

## References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Becker, P. J. & Coppens, P. (1974). *Acta Cryst.* **A30**, 129–147.
- Bergerhoff, G. (1996). *DIAMOND*. University of Bonn, Germany.
- Chevrel, R. & Sergent, M. (1982). *Superconductivity in Ternary Compounds*, Vol. 1, edited by O. Fischer, pp. 25–86. New York: Springer.
- Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
- Johnson, C. K. & Levy, H. A. (1974). *International Tables for X-ray Crystallography*, edited by J. A. Ibers & W. C. Hamilton, Vol. IV, pp. 311–336. Birmingham: Kynoch Press.
- Meulenaer, J. de & Tompa, H. (1965). *Acta Cryst.* **A19**, 1014–1018.
- Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Petříček, V. & Dušek, M. (2000). *JANA2000*. Institute of Physics, Praha, Czech Republic.
- Tarascon, J. M., Waszczak, J. V., Hull, G. W., DiSalvo, F. J. & Blitzer, L. D. (1983). *Solid State Commun.* **47**, 973–979.

**supplementary materials**

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

## The Chevrel phase HgMo<sub>6</sub>S<sub>8</sub>

D. Salloum, P. Gougeon and M. Potel

### Comment

The superconducting compound HgMo<sub>6</sub>S<sub>8</sub> 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<sub>6</sub>S<sub>8</sub> that has been determined from single-crystal X-ray diffraction data. The title compound is isostructural with the hexagonal Chevrel phases *MMo<sub>6</sub>X<sub>8</sub>* where *M* is a large cation (*M* = alkali metal, alkaline earth, lanthanide, actinide *etc.*; *X* = S, Se, Te) [see, for instance, Chevrel & Sergent (1982)]. As a consequence its crystal structure consists of octahedral Mo<sub>6</sub> 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<sub>8</sub> cube (*a*-type ligands). In the structure of HgMo<sub>6</sub>S<sub>8</sub>, a part of the chalcogen atoms of the Mo<sub>6</sub>S<sub>8</sub> unit are shared according to the formula Mo<sub>6</sub>S<sub>2</sub><sup>*i*</sup>S<sub>6/2</sub><sup>*i-a*</sup>S<sub>6/2</sub><sup>*a-i*</sup> to form the three-dimensional Mo—S network. The Mo<sub>6</sub>S<sub>8</sub> cluster unit is centered at Wyckoff position 6*b* ( $\bar{3}$  symmetry). The Mo—Mo distances within the Mo<sub>6</sub> clusters are 2.7184 (3) Å for the intra-triangle distances (distances within the Mo<sub>3</sub> 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<sub>6</sub>S<sub>8</sub> unit is interconnected to 6 Mo<sub>6</sub>S<sub>8</sub> units to form the Mo—S framework. It results from this arrangement that the shortest intercluster Mo1—Mo1 distances between the Mo<sub>6</sub> clusters is 3.2934 (3) Å, indicating only weak metal-metal interaction. The Hg<sup>2+</sup> cations reside in the large eight-coordinate voids formed by the chalcogen atoms from eight different Mo<sub>6</sub>S<sub>8</sub> units. They are covalently bonded to two S2 atoms at a distance of 2.3914 (8) Å.

HgMo<sub>6</sub>S<sub>8</sub> was found to be superconducting at 8 K from DC-susceptibility measurements on a batch of single crystals.

### Experimental

HgMo<sub>6</sub>S<sub>8</sub> was obtained in three steps involving, first, the syntheses of single-crystal of InMo<sub>6</sub>S<sub>8</sub> by solid state reaction, then the preparation of the binary compound Mo<sub>6</sub>S<sub>8</sub> by 'chimie douce' methods and, finally, the synthesis of the title compound by inserting mercury into the Mo<sub>6</sub>S<sub>8</sub> host structure at low temperatures. Single crystals of InMo<sub>6</sub>S<sub>8</sub> were obtained from a stoichiometric mixture of In<sub>2</sub>S<sub>3</sub>, MoS<sub>2</sub> 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<sub>6</sub>S<sub>8</sub> was obtained by oxidation of single-crystals of InMo<sub>6</sub>S<sub>8</sub> 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<sub>3</sub> and I<sub>2</sub> were obtained at the cooler end of the tube. Finally, HgMo<sub>6</sub>S<sub>8</sub> was prepared by diffusion of mercury into crystals of Mo<sub>6</sub>S<sub>8</sub> in a silica glass tube sealed under vacuum at 673 K during 96 h.

## 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  $\text{Hg}_{0.973(3)}\text{Mo}_6\text{S}_8$ .

## Figures

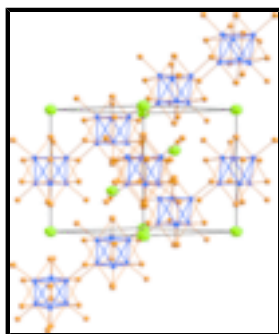


Fig. 1. : View of  $\text{HgMo}_6\text{S}_8$  along  $[110]$ .

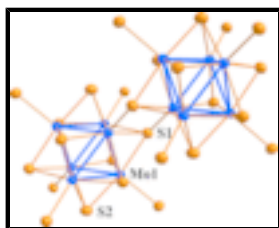


Fig. 2. : Plot showing the atom-numbering scheme and the interunit linkage of the  $(\text{Mo}_6\text{S}_8)\text{S}_6$  cluster units. Displacement ellipsoids are drawn at the 97% probability level.

(I)

### Crystal data

$\text{Hg}_{0.973}\text{Mo}_6\text{S}_8$

$M_r = 1027.3$

Trigonal,  $R\bar{3}$

Hall symbol:  $-R\ 3$

$a = 9.4319(3)\ \text{\AA}$

$b = 9.4319(3)\ \text{\AA}$

$c = 10.7028(3)\ \text{\AA}$

$\alpha = 90^\circ$

$\beta = 90^\circ$

$\gamma = 120^\circ$

$V = 824.57(4)\ \text{\AA}^3$

$Z = 3$

$F_{000} = 1374$

$D_x = 6.204(1)\ \text{Mg m}^{-3}$

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

$0.08 \times 0.07 \times 0.06\ \text{mm}$

*Data collection*

Nonius KappaCCD diffractometer	1121 independent reflections
Radiation source: fine-focus sealed tube	1069 reflections with $I > 2\sigma(I)$
Monochromator: horizontally mounted graphite crystal	$R_{\text{int}} = 0.044$
Detector resolution: 9 pixels $\text{mm}^{-1}$	$\theta_{\text{max}} = 39.8^\circ$
$T = 293$ K	$\theta_{\text{min}} = 3.1^\circ$
$\omega$ - and $\varphi$ -scans	$h = -16 \rightarrow 16$
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	$k = -16 \rightarrow 16$
$T_{\text{min}} = 0.298$ , $T_{\text{max}} = 0.384$	$l = -13 \rightarrow 19$
5784 measured reflections	

*Refinement*

Refinement on $F$	Weighting scheme based on measured s.u.'s $w = 1/\sigma^2(F)$
$R[F^2 > 2\sigma(F^2)] = 0.025$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$wR(F^2) = 0.026$	$\Delta\rho_{\text{max}} = 2.64 \text{ e } \text{\AA}^{-3}$
$S = 1.74$	$\Delta\rho_{\text{min}} = -1.57 \text{ e } \text{\AA}^{-3}$
1121 reflections	Extinction correction: B-C type 1 Lorentzian isotropic (Becker & Coppens, 1974)
31 parameters	Extinction coefficient: 0.020681

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	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 ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 ( $\text{\AA}$ ,  $^\circ$ )*

Hg1—S1	2.3914 (8)	Mo1—Mo1 <sup>ix</sup>	2.7184 (3)
Hg1—S1 <sup>i</sup>	2.3914 (8)	Mo1—Mo1 <sup>x</sup>	2.7515 (3)
Hg1—S2 <sup>ii</sup>	3.2056 (4)	Mo1—Mo1 <sup>xi</sup>	2.7184 (4)

## supplementary materials

Hg1—S2 <sup>iii</sup>	3.2056 (4)	Mo1—Mo1 <sup>xii</sup>	2.7515 (2)
Hg1—S2 <sup>iv</sup>	3.2056 (7)	Mo1—S1	2.4108 (7)
Hg1—S2 <sup>v</sup>	3.2056 (7)	Mo1—S2	2.4236 (6)
Hg1—S2 <sup>vi</sup>	3.2056 (8)	Mo1—S2 <sup>xiii</sup>	2.4896 (8)
Hg1—S2 <sup>vii</sup>	3.2056 (8)	Mo1—S2 <sup>x</sup>	2.4933 (6)
Mo1—Mo1 <sup>viii</sup>	3.8679 (3)	Mo1—S2 <sup>xii</sup>	2.4340 (8)
Mo1—Mo1 <sup>iii</sup>	3.2131 (2)		
S1—Hg1—S1 <sup>i</sup>	180	Mo1 <sup>x</sup> —Mo1—Mo1 <sup>iii</sup>	97.693 (7)
S1—Hg1—S2 <sup>ii</sup>	105.278 (8)	Mo1 <sup>x</sup> —Mo1—Mo1 <sup>ix</sup>	90
S1—Hg1—S2 <sup>iii</sup>	74.722 (8)	Mo1 <sup>x</sup> —Mo1—Mo1 <sup>xi</sup>	60.398 (8)
S1—Hg1—S2 <sup>iv</sup>	105.278 (9)	Mo1 <sup>x</sup> —Mo1—Mo1 <sup>xii</sup>	59.205 (7)
S1—Hg1—S2 <sup>v</sup>	74.722 (9)	Mo1 <sup>x</sup> —Mo1—S1	115.964 (15)
S1—Hg1—S2 <sup>vi</sup>	105.278 (9)	Mo1 <sup>x</sup> —Mo1—S2	55.677 (18)
S1—Hg1—S2 <sup>vii</sup>	74.722 (9)	Mo1 <sup>x</sup> —Mo1—S2 <sup>xiii</sup>	138.626 (14)
S1 <sup>i</sup> —Hg1—S1	180	Mo1 <sup>x</sup> —Mo1—S2 <sup>x</sup>	54.776 (13)
S1 <sup>i</sup> —Hg1—S2 <sup>ii</sup>	74.722 (8)	Mo1 <sup>x</sup> —Mo1—S2 <sup>xii</sup>	114.515 (14)
S1 <sup>i</sup> —Hg1—S2 <sup>iii</sup>	105.278 (8)	Mo1 <sup>xi</sup> —Mo1—Mo1 <sup>iii</sup>	96.739 (8)
S1 <sup>i</sup> —Hg1—S2 <sup>iv</sup>	74.722 (9)	Mo1 <sup>xi</sup> —Mo1—Mo1 <sup>ix</sup>	60.000 (8)
S1 <sup>i</sup> —Hg1—S2 <sup>v</sup>	105.278 (9)	Mo1 <sup>xi</sup> —Mo1—Mo1 <sup>x</sup>	60.398 (8)
S1 <sup>i</sup> —Hg1—S2 <sup>vi</sup>	74.722 (9)	Mo1 <sup>xi</sup> —Mo1—Mo1 <sup>xii</sup>	90
S1 <sup>i</sup> —Hg1—S2 <sup>vii</sup>	105.278 (9)	Mo1 <sup>xi</sup> —Mo1—S1	55.682 (12)
S2 <sup>ii</sup> —Hg1—S2 <sup>iii</sup>	180	Mo1 <sup>xi</sup> —Mo1—S2	116.065 (18)
S2 <sup>ii</sup> —Hg1—S2 <sup>iv</sup>	113.319 (18)	Mo1 <sup>xi</sup> —Mo1—S2 <sup>xiii</sup>	135.971 (18)
S2 <sup>ii</sup> —Hg1—S2 <sup>v</sup>	66.681 (18)	Mo1 <sup>xi</sup> —Mo1—S2 <sup>x</sup>	55.48 (2)
S2 <sup>ii</sup> —Hg1—S2 <sup>vi</sup>	113.319 (17)	Mo1 <sup>xi</sup> —Mo1—S2 <sup>xii</sup>	117.362 (19)
S2 <sup>ii</sup> —Hg1—S2 <sup>vii</sup>	66.681 (17)	Mo1 <sup>xii</sup> —Mo1—Mo1 <sup>iii</sup>	148.317 (7)
S2 <sup>iii</sup> —Hg1—S2 <sup>ii</sup>	180	Mo1 <sup>xii</sup> —Mo1—Mo1 <sup>ix</sup>	60.398 (6)
S2 <sup>iii</sup> —Hg1—S2 <sup>iv</sup>	66.681 (18)	Mo1 <sup>xii</sup> —Mo1—Mo1 <sup>x</sup>	59.205 (7)
S2 <sup>iii</sup> —Hg1—S2 <sup>v</sup>	113.319 (18)	Mo1 <sup>xii</sup> —Mo1—Mo1 <sup>xi</sup>	90
S2 <sup>iii</sup> —Hg1—S2 <sup>vi</sup>	66.681 (17)	Mo1 <sup>xii</sup> —Mo1—S1	115.964 (13)
S2 <sup>iii</sup> —Hg1—S2 <sup>vii</sup>	113.319 (17)	Mo1 <sup>xii</sup> —Mo1—S2	57.184 (12)
S2 <sup>iv</sup> —Hg1—S2 <sup>ii</sup>	113.319 (18)	Mo1 <sup>xii</sup> —Mo1—S2 <sup>xiii</sup>	133.837 (19)
S2 <sup>iv</sup> —Hg1—S2 <sup>iii</sup>	66.681 (18)	Mo1 <sup>xii</sup> —Mo1—S2 <sup>x</sup>	113.894 (15)
S2 <sup>iv</sup> —Hg1—S2 <sup>v</sup>	180	Mo1 <sup>xii</sup> —Mo1—S2 <sup>xii</sup>	55.318 (14)
S2 <sup>iv</sup> —Hg1—S2 <sup>vi</sup>	113.319 (19)	S1—Mo1—S2	170.65 (2)
S2 <sup>iv</sup> —Hg1—S2 <sup>vii</sup>	66.681 (19)	S1—Mo1—S2 <sup>xiii</sup>	93.53 (2)
S2 <sup>v</sup> —Hg1—S2 <sup>ii</sup>	66.681 (18)	S1—Mo1—S2 <sup>x</sup>	90.323 (17)
S2 <sup>v</sup> —Hg1—S2 <sup>iii</sup>	113.319 (18)	S1—Mo1—S2 <sup>xii</sup>	91.758 (14)
S2 <sup>v</sup> —Hg1—S2 <sup>iv</sup>	180	S2—Mo1—S2 <sup>xiii</sup>	95.79 (2)
S2 <sup>v</sup> —Hg1—S2 <sup>vi</sup>	66.681 (19)	S2—Mo1—S2 <sup>x</sup>	87.39 (2)

S2 <sup>v</sup> —Hg1—S2 <sup>vii</sup>	113.319 (19)	S2—Mo1—S2 <sup>xii</sup>	88.750 (19)
S2 <sup>vi</sup> —Hg1—S2 <sup>ii</sup>	113.319 (17)	S2 <sup>xiii</sup> —Mo1—S2	95.79 (2)
S2 <sup>vi</sup> —Hg1—S2 <sup>iii</sup>	66.681 (17)	S2 <sup>xiii</sup> —Mo1—S2 <sup>x</sup>	99.70 (2)
S2 <sup>vi</sup> —Hg1—S2 <sup>iv</sup>	113.319 (19)	S2 <sup>xiii</sup> —Mo1—S2 <sup>xii</sup>	91.39 (2)
S2 <sup>vi</sup> —Hg1—S2 <sup>v</sup>	66.681 (19)	S2 <sup>x</sup> —Mo1—S2	87.39 (2)
S2 <sup>vi</sup> —Hg1—S2 <sup>vii</sup>	180	S2 <sup>x</sup> —Mo1—S2 <sup>xiii</sup>	99.70 (2)
S2 <sup>vii</sup> —Hg1—S2 <sup>ii</sup>	66.681 (17)	S2 <sup>x</sup> —Mo1—S2 <sup>xii</sup>	168.58 (2)
S2 <sup>vii</sup> —Hg1—S2 <sup>iii</sup>	113.319 (17)	S2 <sup>xii</sup> —Mo1—S2	88.750 (19)
S2 <sup>vii</sup> —Hg1—S2 <sup>iv</sup>	66.681 (19)	S2 <sup>xii</sup> —Mo1—S2 <sup>xiii</sup>	91.39 (2)
S2 <sup>vii</sup> —Hg1—S2 <sup>v</sup>	113.319 (19)	S2 <sup>xii</sup> —Mo1—S2 <sup>x</sup>	168.58 (2)
S2 <sup>vii</sup> —Hg1—S2 <sup>vi</sup>	180	Hg1—S1—Mo1	139.382 (14)
Mo1 <sup>viii</sup> —Mo1—Mo1 <sup>iii</sup>	133.459 (8)	Hg1—S1—Mo1 <sup>ix</sup>	139.382 (13)
Mo1 <sup>viii</sup> —Mo1—S1	85.136 (14)	Hg1—S1—Mo1 <sup>xi</sup>	139.382 (14)
Mo1 <sup>viii</sup> —Mo1—S2	85.600 (16)	Mo1—S1—Mo1 <sup>ix</sup>	68.64 (2)
Mo1 <sup>viii</sup> —Mo1—S2 <sup>xiii</sup>	176.394 (13)	Mo1—S1—Mo1 <sup>xi</sup>	68.64 (2)
Mo1 <sup>viii</sup> —Mo1—S2 <sup>x</sup>	83.677 (18)	Mo1 <sup>ix</sup> —S1—Mo1	68.64 (2)
Mo1 <sup>viii</sup> —Mo1—S2 <sup>xii</sup>	85.310 (16)	Mo1 <sup>ix</sup> —S1—Mo1 <sup>xi</sup>	68.64 (2)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>viii</sup>	133.459 (8)	Mo1 <sup>xi</sup> —S1—Mo1	68.64 (2)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>ix</sup>	147.479 (10)	Mo1 <sup>xi</sup> —S1—Mo1 <sup>ix</sup>	68.64 (2)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>x</sup>	97.693 (7)	Hg1 <sup>xiv</sup> —S2—Mo1	125.450 (18)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>xi</sup>	96.739 (8)	Hg1 <sup>xiv</sup> —S2—Mo1 <sup>x</sup>	98.407 (18)
Mo1 <sup>iii</sup> —Mo1—Mo1 <sup>xii</sup>	148.317 (7)	Hg1 <sup>xiv</sup> —S2—Mo1 <sup>xv</sup>	97.225 (18)
Mo1 <sup>iii</sup> —Mo1—S1	92.988 (11)	Hg1 <sup>xiv</sup> —S2—Mo1 <sup>xii</sup>	156.59 (2)
Mo1 <sup>iii</sup> —Mo1—S2	92.457 (12)	Mo1—S2—Mo1 <sup>x</sup>	69.005 (19)
Mo1 <sup>iii</sup> —Mo1—S2 <sup>xiii</sup>	49.898 (13)	Mo1—S2—Mo1 <sup>xv</sup>	132.74 (2)
Mo1 <sup>iii</sup> —Mo1—S2 <sup>x</sup>	49.797 (18)	Mo1—S2—Mo1 <sup>xii</sup>	68.041 (15)
Mo1 <sup>iii</sup> —Mo1—S2 <sup>xii</sup>	141.203 (18)	Mo1 <sup>x</sup> —S2—Mo1	69.005 (19)
Mo1 <sup>ix</sup> —Mo1—Mo1 <sup>iii</sup>	147.479 (10)	Mo1 <sup>x</sup> —S2—Mo1 <sup>xv</sup>	129.09 (2)
Mo1 <sup>ix</sup> —Mo1—Mo1 <sup>x</sup>	90	Mo1 <sup>x</sup> —S2—Mo1 <sup>xii</sup>	66.955 (19)
Mo1 <sup>ix</sup> —Mo1—Mo1 <sup>xi</sup>	60.000 (8)	Mo1 <sup>xv</sup> —S2—Mo1	132.74 (2)
Mo1 <sup>ix</sup> —Mo1—Mo1 <sup>xii</sup>	60.398 (6)	Mo1 <sup>xv</sup> —S2—Mo1 <sup>x</sup>	129.09 (2)
Mo1 <sup>ix</sup> —Mo1—S1	55.682 (11)	Mo1 <sup>xv</sup> —S2—Mo1 <sup>xii</sup>	80.305 (15)
Mo1 <sup>ix</sup> —Mo1—S2	117.489 (13)	Mo1 <sup>xii</sup> —S2—Mo1	68.041 (15)
Mo1 <sup>ix</sup> —Mo1—S2 <sup>xiii</sup>	131.337 (14)	Mo1 <sup>xii</sup> —S2—Mo1 <sup>x</sup>	66.955 (19)
Mo1 <sup>ix</sup> —Mo1—S2 <sup>x</sup>	115.28 (2)	Mo1 <sup>xii</sup> —S2—Mo1 <sup>xv</sup>	80.305 (15)
Mo1 <sup>ix</sup> —Mo1—S2 <sup>xii</sup>	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)  $-x+y+1/3, -x-1/3, z-1/3$ .

Fig. 1

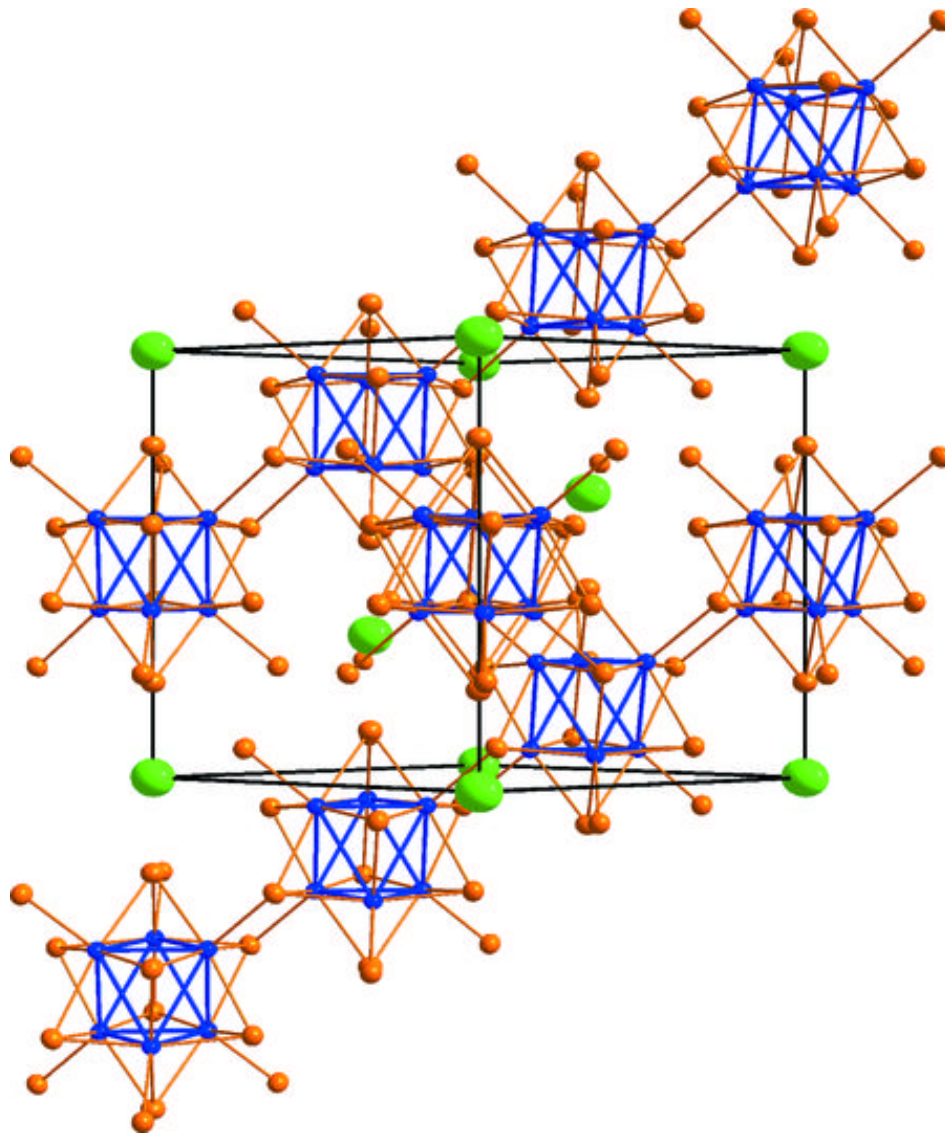


Fig. 2

