

Dicaesium hexamercury heptasulfide

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 Key indicators: single-crystal X-ray study; $T = 215$ K; mean $\sigma(\text{Hg}-\text{S}) = 0.005$ Å; R factor = 0.034; wR factor = 0.082; data-to-parameter ratio = 22.2.

The title compound, $\text{Cs}_2\text{Hg}_6\text{S}_7$, crystallizes in a new structure type that is closely related to that of $\text{K}_2\text{Zn}_6\text{O}_7$. The structure comprises a three-dimensional mercury sulfide network that is composed of channels. These channels, which are along [001], are of two different diameters. The crystal structure contains one Cs, two Hg, and three S atoms in the asymmetric unit. The Cs, one Hg, and one S atom are at sites of symmetry m , whereas a second S atom is at a site of symmetry $2mm$. The Hg atoms are bound to the S atoms in both three- and four-coordinate geometries. The caesium cations occupy the central spaces of the larger diameter channels and exhibit a coordination number of 7.

Related literature

For literature on related alkali-metal mercury sulfides, see: Sommer & Hoppe (1978) for A_6HgS_4 ($A = \text{K}, \text{Rb}$); Klepp & Prager (1992) for A_2HgS_2 ($A = \text{Na}, \text{K}$); Klepp (1992) for $\text{Na}_2\text{Hg}_3\text{S}_4$; Kanatzidis & Park (1990) for $\text{K}_2\text{Hg}_5\text{S}_4$ and $\text{K}_2\text{Hg}_6\text{S}_7$. For literature on other compounds with Hg—S or Cs—S bonds, see: Gulay *et al.* (2002); Rad & Hoppe (1981); Iwasaki (1973); Kinoshita *et al.* (1985); Bronger & Hendriks (1980). The isoformular, but not isotypic, compound $\text{K}_2\text{Zn}_6\text{O}_7$ was reported by Wambach & Hoppe (1978). For synthetic details, see: Sunshine *et al.* (1987). For computational details, see: Brown & Altermatt (1985); Gelato & Parthé (1987); Le Page (1988); Brese & O'Keeffe (1991); Spek (2003).

Experimental

Crystal data

$\text{Cs}_2\text{Hg}_6\text{S}_7$	$Z = 2$
$M_r = 1693.78$	Mo $K\alpha$ radiation
Tetragonal, $P4_2nm$	$\mu = 60.56 \text{ mm}^{-1}$
$a = 14.063$ (3) Å	$T = 215$ (2) K
$c = 4.1895$ (18) Å	$0.44 \times 0.06 \times 0.04 \text{ mm}$
$V = 828.6$ (4) Å ³	

Data collection

Bruker SMART 1000 CCD diffractometer	8644 measured reflections
Absorption correction: face-indexed, numerical (<i>SADABS</i> ; Sheldrick, 2006)	956 independent reflections
$T_{\min} = 0.011$, $T_{\max} = 0.131$	907 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.052$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	$\Delta\rho_{\text{max}} = 2.17 \text{ e \AA}^{-3}$
$wR(F^2) = 0.082$	$\Delta\rho_{\text{min}} = -2.29 \text{ e \AA}^{-3}$
$S = 1.23$	Absolute structure: Flack (1983), 389 Friedel pairs
956 reflections	Flack parameter: 0.00 (3)
43 parameters	
1 restraint	

Table 1

Selected geometric parameters (Å, °).

Hg1—S1	2.488 (4)	Cs1—S1 ^v	3.526 (5)
Hg1—S1 ⁱ	2.540 (5)	Cs1—S1 ⁱⁱ	3.526 (5)
Hg1—S1 ⁱⁱⁱ	2.549 (5)	Cs1—S1 ^{vi}	3.561 (5)
Hg1—S3 ⁱⁱⁱ	2.7754 (15)	Cs1—S1 ⁱ	3.561 (5)
Hg2—S3	2.367 (7)	Cs1—S2 ^{vii}	3.566 (4)
Hg2—S2	2.377 (5)	Cs1—S3 ^{iv}	3.609 (7)
Hg2—S3 ^{iv}	3.004 (7)	Cs1—S3	3.627 (7)
S1—Hg1—S1 ⁱ	121.0 (2)	S1 ⁱⁱ —Hg1—S3 ⁱⁱⁱ	95.74 (17)
S1—Hg1—S1 ⁱⁱⁱ	120.6 (2)	S3—Hg2—S2	168.5 (3)
S1 ⁱ —Hg1—S1 ⁱⁱⁱ	110.83 (15)	S3—Hg2—S3 ^{iv}	101.9 (2)
S1—Hg1—S3 ⁱⁱⁱ	104.78 (15)	S2—Hg2—S3 ^{iv}	89.7 (2)
S1 ⁱ —Hg1—S3 ⁱⁱⁱ	96.43 (18)		

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *APEX2* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalMaker* (Palmer, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2184).

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supplementary materials

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Comment

Four structure types are found in alkali metal-mercury-sulfur ternary systems: $A_6\text{HgS}_4$ ($A = \text{K}, \text{Rb}$) exhibit discrete HgS_4 tetrahedra with intercalated alkali-metal cations (Sommer & Hoppe, 1978). $A_2\text{HgS}_2$ ($A = \text{Na}, \text{K}$) possess nearly linear HgS_2 units with alkali-metal cations occupying the voids (Klepp & Prager, 1992). The compounds $\text{Na}_2\text{Hg}_3\text{S}_4$ (Klepp, 1992) and $\text{K}_2\text{Hg}_3\text{S}_4$ (Kanatzidis & Park, 1990) feature infinite $[\text{Hg}_3\text{S}_4]^{2-}$ units parallel to (100) separated by alkali-metal cations. $\text{K}_2\text{Hg}_6\text{S}_7$ has a three-dimensional mercury sulfide network composed of two types of channels, with the potassium cations occupying the spaces in the larger-diameter channels (Kanatzidis & Park, 1990).

Fig. 1 shows the unit cell of $\text{Cs}_2\text{Hg}_6\text{S}_7$. Similar to $\text{K}_2\text{Hg}_6\text{S}_7$, there is a three-dimensional mercury sulfide network containing two types of channels along [001]. There are two types of coordination geometries for the mercury atoms: Hg1 is four-coordinate with a distorted tetrahedral geometry and Hg2 is three-coordinate with a T-shaped planar geometry. The Hg1—S bond distances of 2.488 (4)-2.775 (2) Å are comparable to those of 2.345 (8)-2.718 (4) Å in $\text{K}_2\text{Hg}_6\text{S}_7$. The Hg2—S bond distances are 2.367 (7), 2.377 (5), and 3.004 (7) Å. In $\text{K}_2\text{Hg}_6\text{S}_7$, the Hg2 atom is considered to have a two-coordinate, nearly linear geometry. The Hg2 atom in $\text{Cs}_2\text{Hg}_6\text{S}_7$ can also be viewed as having an approximately linear bonding environment if the Hg2—S coordination distance of 3.004 (7) Å is considered to be non-bonding. However, there are some examples in the literature of longer than expected Hg—S bonds in extended solid-state structures, including 2.92 (1) Å in Hg_4SiS_6 (Gulay *et al.*, 2002), and 2.98 (1) Å in BaHgS_2 (Rad & Hoppe, 1981). Long Hg—S bond distances of greater than 2.9 Å are more common in coordination compounds, including 2.965 (4) Å in $\text{Hg}(\text{S}_2\text{CNEt}_2)_2$ (Iwasaki, 1973), 3.137 (6) Å in $\text{Hg}_2(\text{S}_2\text{CNEt}_2)_4$ (Iwasaki, 1973), and 2.991 (3) Å and 3.322 (4) Å in $[\text{CoHg}(\text{SCN})_4\{\text{P}(\text{C}_6\text{H}_5)_3\}_2]_2$ (Kinoshita *et al.*, 1985). Therefore, we consider the Hg2 atom in $\text{Cs}_2\text{Hg}_6\text{S}_7$ to be three-coordinate with a T-shaped planar geometry. The Cs1 atoms, found in the centers of the larger-diameter channels, are seven-coordinate, with Cs—S distances of 3.526 (5)-3.627 (7) Å, as compared to 3.595 (7)-3.701 (6) Å in $\text{Cs}_2\text{Zn}_3\text{S}_4$ (Bronger & Hendriks, 1980).

Because there is no S—S bonding in $\text{Cs}_2\text{Hg}_6\text{S}_7$, a formal oxidation state of -II can be assigned to the S atoms. Bond valence sums (Brown & Altermatt, 1985; Brese & O'Keeffe, 1991) of Hg1 = 1.95, Hg2 = 1.84, and Cs1 = 1.13 confirm the formal oxidation states of +II for both Hg atoms, and +I for Cs.

Although they possess structural similarities, $\text{Cs}_2\text{Hg}_6\text{S}_7$ and $\text{K}_2\text{Hg}_6\text{S}_7$ are not isostructural. $\text{Cs}_2\text{Hg}_6\text{S}_7$ belongs to space group $P4_2nm$ and $\text{K}_2\text{Hg}_6\text{S}_7$ belongs to space group $P\bar{4}2_1m$. Another related compound is $\text{K}_2\text{Zn}_6\text{O}_7$, which crystallizes in space group $P4_2nm$ (Wambach & Hoppe, 1978). However, the *ADDSYM* algorithm (Le Page, 1988) in *PLATON* (Spek, 2003) suggests that $\text{K}_2\text{Zn}_6\text{O}_7$ properly belongs to space group $P4_2/mnm$. Apparently, $\text{Cs}_2\text{Hg}_6\text{S}_7$ is not isostructural to $\text{K}_2\text{Zn}_6\text{O}_7$ and instead crystallizes in a new structure type.

Experimental

Cs₂Hg₆S₇ was initially obtained in an attempt to produce a Cs/Hg/U/S quaternary phase. Cs₂Hg₆S₇ was then synthesized rationally from a solid-state reaction of Cs₂S₃ (0.13 mmol), HgS (Alfa Aesar, 0.21 mmol), and S (Mallinckrodt, 99.6%, 0.44 mmol). CsI (Aldrich, 99.9%, 0.34 mmol) was added to aid in the crystallization of the final product. The Cs₂S₃ reactive flux (Sunshine *et al.*, 1987) was prepared by the stoichiometric reaction of Cs (Strem Chemicals, 99.5%) and S in liquid NH₃ at 194 K. The reactants were loaded into a fused-silica tube under an Ar atmosphere in a glove box. The tube was evacuated to 10⁻⁴ Torr, sealed, and then placed in a computer-controlled furnace. The sample was heated to 1123 K in 24 hours, kept at 1123 K for 120 h, cooled at 5 K h⁻¹ to 473 K, and then cooled to 293 K in 2 hours. The resulting black needles were washed with *N,N*-dimethylformamide. The yield was about 80% based on Hg.

Refinement

The structure was standardized by means of the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak is 1.60 Å from atom Hg1 and the deepest hole is 1.03 Å from atom S3.

Figures

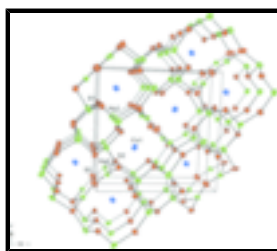


Fig. 1. A view down [001] of the unit cell of Cs₂Hg₆S₇, with displacement ellipsoids at the 95% probability level.

Dicaesium hexamercury heptasulfide

Crystal data

Cs₂Hg₆S₇

$M_r = 1693.78$

Tetragonal, $P4_2nm$

Hall symbol: P 4n -2n

$a = 14.063 (3) \text{ \AA}$

$b = 14.063 (3) \text{ \AA}$

$c = 4.1895 (18) \text{ \AA}$

$\alpha = 90^\circ$

$\beta = 90^\circ$

$\gamma = 90^\circ$

$V = 828.6 (4) \text{ \AA}^3$

$Z = 2$

$F_{000} = 1404$

$D_x = 6.789 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 5893 reflections

$\theta = 2.9\text{--}28.1^\circ$

$\mu = 60.56 \text{ mm}^{-1}$

$T = 215 (2) \text{ K}$

Needle, black

$0.44 \times 0.06 \times 0.04 \text{ mm}$

Data collection

Bruker SMART 1000 CCD diffractometer	956 independent reflections
Radiation source: fine-focus sealed tube	907 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.052$
$T = 215(2)$ K	$\theta_{\text{max}} = 28.1^\circ$
ω scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: numerical (SADABS; Sheldrick, 2006)	$h = -17 \rightarrow 17$
$T_{\text{min}} = 0.011$, $T_{\text{max}} = 0.131$	$k = -17 \rightarrow 17$
8644 measured reflections	$l = -5 \rightarrow 5$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2 + 40.9819P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.082$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.23$	$\Delta\rho_{\text{max}} = 2.17 \text{ e } \text{\AA}^{-3}$
956 reflections	$\Delta\rho_{\text{min}} = -2.29 \text{ e } \text{\AA}^{-3}$
43 parameters	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.00320 (17)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 389 Friedel pairs Flack parameter: 0.00 (3)

Special details

Experimental. The absorption correction program used the face indices and crystal dimensions that were supplied.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	0.15251 (5)	0.57410 (5)	0.22339 (19)	0.0216 (2)
Hg2	0.09922 (5)	0.09922 (5)	0.3162 (3)	0.0189 (3)
Cs1	0.33108 (8)	0.33108 (8)	0.2149 (5)	0.0197 (3)
S1	0.0207 (3)	0.6920 (3)	0.2220 (13)	0.0151 (7)
S2	0.0000	0.0000	0.000 (2)	0.0193 (19)
S3	0.1828 (3)	0.1828 (3)	0.7187 (18)	0.0153 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.0248 (4)	0.0215 (4)	0.0184 (4)	0.0052 (3)	0.0002 (3)	-0.0002 (3)
Hg2	0.0180 (3)	0.0180 (3)	0.0206 (5)	-0.0015 (4)	-0.0032 (3)	-0.0032 (3)

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Cs1	0.0216 (5)	0.0216 (5)	0.0157 (7)	0.0037 (5)	-0.0013 (6)	-0.0013 (6)
S1	0.0134 (18)	0.0160 (18)	0.0158 (18)	-0.0006 (14)	-0.0002 (19)	-0.0017 (19)
S2	0.024 (3)	0.024 (3)	0.011 (4)	-0.006 (4)	0.000	0.000
S3	0.0154 (15)	0.0154 (15)	0.015 (2)	0.002 (2)	-0.003 (2)	-0.003 (2)

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

Hg1—S1	2.488 (4)	Cs1—S2 ^{iv}	3.566 (4)
Hg1—S1 ⁱ	2.540 (5)	Cs1—S3 ^v	3.609 (7)
Hg1—S1 ⁱⁱ	2.549 (5)	Cs1—S3	3.627 (7)
Hg1—S3 ⁱⁱⁱ	2.7754 (15)	Cs1—Hg1 ^{viii}	4.1659 (17)
Hg1—Cs1 ^{iv}	4.1659 (17)	Cs1—Hg1 ⁱⁱ	4.1659 (17)
Hg1—Cs1 ⁱⁱⁱ	4.2013 (18)	Cs1—Cs1 ^x	4.1895 (18)
Hg1—Cs1	4.2412 (12)	Cs1—Cs1 ^v	4.1895 (18)
Hg2—S3	2.367 (7)	Cs1—Hg1 ⁱ	4.2013 (18)
Hg2—S2	2.377 (5)	S1—Hg1 ⁱⁱⁱ	2.540 (5)
Hg2—S3 ^v	3.004 (7)	S1—Hg1 ^{iv}	2.549 (5)
Hg2—Cs1 ⁱ	4.2392 (19)	S1—Cs1 ^{iv}	3.526 (5)
Hg2—Cs1 ^{vi}	4.2392 (18)	S1—Cs1 ⁱⁱⁱ	3.561 (5)
Hg2—Cs1	4.631 (2)	S2—Hg2 ^{xi}	2.377 (5)
Hg2—Cs1 ⁱⁱ	4.640 (2)	S2—Cs1 ⁱⁱ	3.566 (4)
Hg2—Cs1 ^{vii}	4.640 (2)	S2—Cs1 ^{vii}	3.566 (4)
Cs1—S1 ^{viii}	3.526 (5)	S3—Hg1 ^{ix}	2.7754 (14)
Cs1—S1 ⁱⁱ	3.526 (5)	S3—Hg1 ⁱ	2.7754 (14)
Cs1—S1 ^{ix}	3.561 (5)	S3—Hg2 ^x	3.004 (7)
Cs1—S1 ⁱ	3.561 (5)	S3—Cs1 ^x	3.609 (7)
S1—Hg1—S1 ⁱ	121.0 (2)	S1 ^{ix} —Cs1—S2 ^{iv}	77.06 (11)
S1—Hg1—S1 ⁱⁱ	120.6 (2)	S1 ⁱ —Cs1—S2 ^{iv}	77.06 (11)
S1 ⁱ —Hg1—S1 ⁱⁱ	110.83 (15)	S1 ^{viii} —Cs1—S3 ^v	71.57 (10)
S1—Hg1—S3 ⁱⁱⁱ	104.78 (15)	S1 ⁱⁱ —Cs1—S3 ^v	71.57 (10)
S1 ⁱ —Hg1—S3 ⁱⁱⁱ	96.43 (18)	S1 ^{ix} —Cs1—S3 ^v	111.39 (9)
S1 ⁱⁱ —Hg1—S3 ⁱⁱⁱ	95.74 (17)	S1 ⁱ —Cs1—S3 ^v	111.39 (9)
S1—Hg1—Cs1 ^{iv}	57.59 (10)	S2 ^{iv} —Cs1—S3 ^v	164.39 (19)
S1 ⁱ —Hg1—Cs1 ^{iv}	92.09 (11)	S1 ^{viii} —Cs1—S3	111.21 (9)
S1 ⁱⁱ —Hg1—Cs1 ^{iv}	148.09 (10)	S1 ⁱⁱ —Cs1—S3	111.21 (9)
S3 ⁱⁱⁱ —Hg1—Cs1 ^{iv}	58.64 (13)	S1 ^{ix} —Cs1—S3	70.96 (10)
S1—Hg1—Cs1 ⁱⁱⁱ	57.74 (11)	S1 ⁱ —Cs1—S3	70.96 (10)
S1 ⁱ —Hg1—Cs1 ⁱⁱⁱ	148.92 (10)	S2 ^{iv} —Cs1—S3	124.85 (19)
S1 ⁱⁱ —Hg1—Cs1 ⁱⁱⁱ	91.15 (11)	S3 ^v —Cs1—S3	70.76 (11)
S3 ⁱⁱⁱ —Hg1—Cs1 ⁱⁱⁱ	58.46 (14)	Hg1 ^{viii} —Cs1—Hg1 ⁱⁱ	81.48 (4)
Cs1 ^{iv} —Hg1—Cs1 ⁱⁱⁱ	60.09 (3)	S1 ^{viii} —Cs1—Hg1 ⁱ	146.72 (8)
S1—Hg1—Cs1	168.11 (10)	S1 ⁱⁱ —Cs1—Hg1 ⁱ	77.73 (8)

S1 ⁱ —Hg1—Cs1	56.93 (10)	S1 ^{ix} —Cs1—Hg1 ⁱ	103.37 (9)
S1 ⁱⁱ —Hg1—Cs1	56.13 (10)	S1 ⁱ —Cs1—Hg1 ⁱ	36.20 (6)
S3 ⁱⁱⁱ —Hg1—Cs1	87.09 (12)	S2 ^{iv} —Cs1—Hg1 ⁱ	111.51 (11)
Cs1 ^{iv} —Hg1—Cs1	132.09 (4)	S3 ^v —Cs1—Hg1 ⁱ	80.02 (9)
Cs1 ⁱⁱⁱ —Hg1—Cs1	131.02 (4)	S3—Cs1—Hg1 ⁱ	40.70 (2)
S3—Hg2—S2	168.5 (3)	Hg1 ^{viii} —Cs1—Hg1 ⁱ	110.24 (4)
S3—Hg2—S3 ^v	101.9 (2)	Hg1 ⁱⁱ —Cs1—Hg1 ⁱ	60.09 (3)
S2—Hg2—S3 ^v	89.7 (2)	Cs1 ^x —Cs1—Hg1 ⁱ	59.53 (3)
S3—Hg2—Cs1 ⁱ	92.64 (11)	Cs1 ^v —Cs1—Hg1 ⁱ	120.47 (3)
S2—Hg2—Cs1 ⁱ	80.40 (11)	Hg1—S1—Hg1 ⁱⁱⁱ	104.31 (17)
S3 ^v —Hg2—Cs1 ⁱ	125.85 (4)	Hg1—S1—Hg1 ^{iv}	104.03 (17)
S3—Hg2—Cs1 ^{vi}	92.64 (11)	Hg1 ⁱⁱⁱ —S1—Hg1 ^{iv}	110.83 (15)
S2—Hg2—Cs1 ^{vi}	80.40 (11)	Hg1—S1—Cs1 ^{iv}	85.86 (12)
S3 ^v —Hg2—Cs1 ^{vi}	125.85 (4)	Hg1 ⁱⁱⁱ —S1—Cs1 ^{iv}	155.98 (17)
Cs1 ⁱ —Hg2—Cs1 ^{vi}	104.84 (5)	Hg1 ^{iv} —S1—Cs1 ^{iv}	86.99 (14)
S3—Hg2—Cs1	50.68 (17)	Hg1—S1—Cs1 ⁱⁱⁱ	86.05 (12)
S2—Hg2—Cs1	140.87 (19)	Hg1 ⁱⁱⁱ —S1—Cs1 ⁱⁱⁱ	86.37 (14)
S3 ^v —Hg2—Cs1	51.17 (12)	Hg1 ^{iv} —S1—Cs1 ⁱⁱⁱ	156.55 (16)
Cs1 ⁱ —Hg2—Cs1	119.97 (2)	Cs1 ^{iv} —S1—Cs1 ⁱⁱⁱ	72.47 (8)
Cs1 ^{vi} —Hg2—Cs1	119.97 (2)	Hg2—S2—Hg2 ^{xi}	112.2 (4)
S3—Hg2—Cs1 ⁱⁱ	133.26 (3)	Hg2—S2—Cs1 ⁱⁱ	100.76 (3)
S2—Hg2—Cs1 ⁱⁱ	49.02 (6)	Hg2 ^{xi} —S2—Cs1 ⁱⁱ	100.76 (3)
S3 ^v —Hg2—Cs1 ⁱⁱ	77.46 (8)	Hg2—S2—Cs1 ^{vii}	100.76 (3)
Cs1 ⁱ —Hg2—Cs1 ⁱⁱ	56.09 (3)	Hg2 ^{xi} —S2—Cs1 ^{vii}	100.76 (3)
Cs1 ^{vi} —Hg2—Cs1 ⁱⁱ	126.15 (3)	Cs1 ⁱⁱ —S2—Cs1 ^{vii}	140.9 (3)
Cs1—Hg2—Cs1 ⁱⁱ	111.95 (3)	Hg2—S3—Hg1 ^{ix}	98.40 (15)
S3—Hg2—Cs1 ^{vii}	133.26 (3)	Hg2—S3—Hg1 ⁱ	98.40 (15)
S2—Hg2—Cs1 ^{vii}	49.02 (6)	Hg1 ^{ix} —S3—Hg1 ⁱ	156.8 (2)
S3 ^v —Hg2—Cs1 ^{vii}	77.46 (8)	Hg2—S3—Hg2 ^x	101.9 (2)
Cs1 ⁱ —Hg2—Cs1 ^{vii}	126.15 (3)	Hg1 ^{ix} —S3—Hg2 ^x	96.04 (16)
Cs1 ^{vi} —Hg2—Cs1 ^{vii}	56.09 (3)	Hg1 ⁱ —S3—Hg2 ^x	96.04 (16)
Cs1—Hg2—Cs1 ^{vii}	111.95 (3)	Hg2—S3—Cs1 ^x	169.7 (3)
Cs1 ⁱⁱ —Hg2—Cs1 ^{vii}	92.79 (5)	Hg1 ^{ix} —S3—Cs1 ^x	80.31 (13)
S1 ^{viii} —Cs1—S1 ⁱⁱ	108.22 (17)	Hg1 ⁱ —S3—Cs1 ^x	80.31 (13)
S1 ^{viii} —Cs1—S1 ^{ix}	72.47 (8)	Hg2 ^x —S3—Cs1 ^x	88.40 (19)
S1 ⁱⁱ —Cs1—S1 ^{ix}	176.94 (13)	Hg2—S3—Cs1	99.0 (2)
S1 ^{viii} —Cs1—S1 ⁱ	176.94 (13)	Hg1 ^{ix} —S3—Cs1	80.83 (13)
S1 ⁱⁱ —Cs1—S1 ⁱ	72.47 (8)	Hg1 ⁱ —S3—Cs1	80.83 (13)
S1 ^{ix} —Cs1—S1 ⁱ	106.68 (16)	Hg2 ^x —S3—Cs1	159.2 (2)
S1 ^{viii} —Cs1—S2 ^{iv}	99.89 (11)	Cs1 ^x —S3—Cs1	70.76 (11)
S1 ⁱⁱ —Cs1—S2 ^{iv}	99.89 (11)		

supplementary materials

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

Fig. 1

