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## Key indicators

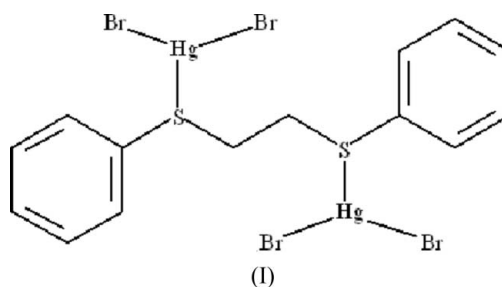
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.011\text{ \AA}$   
 $R$  factor = 0.037  
 $wR$  factor = 0.098  
Data-to-parameter ratio = 19.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>. $[\mu\text{-}1,2\text{-Bis(phenylsulfanyl)ethane-}\kappa^2\text{S:S}']\text{-bis[dibromomercury(II)]}$ 

The title complex,  $[\text{Hg}_2\text{Br}_4(\text{C}_{14}\text{H}_{14}\text{S}_2)]$ , has a dinuclear structure with one 1,2-bis(phenylsulfanyl)ethane ligand linking two  $\text{HgBr}_2$  units, in which the  $\text{Hg}^{\text{II}}$  center adopts a near T-shape coordination geometry formed by two  $\text{Br}^-$  anions and one S atom of 1,2-bis(phenylsulfanyl)ethane. There is a crystallographic inversion center at the mid-point of the central C—C bond. In the crystal structure, when the Hg—Br weak interactions are considered, the dinuclear structure expands into a three-dimensional framework.

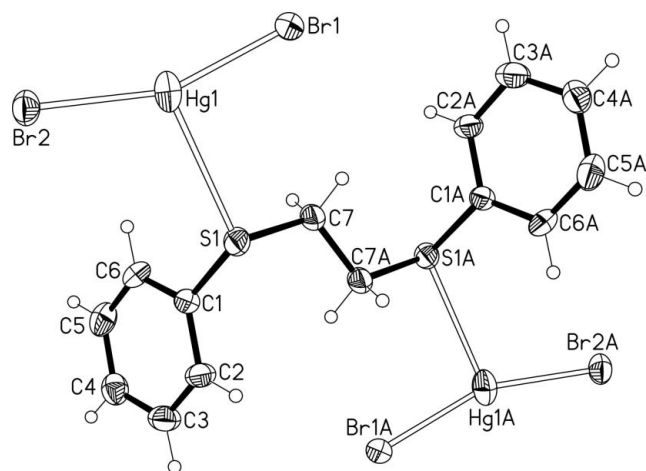
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## Comment

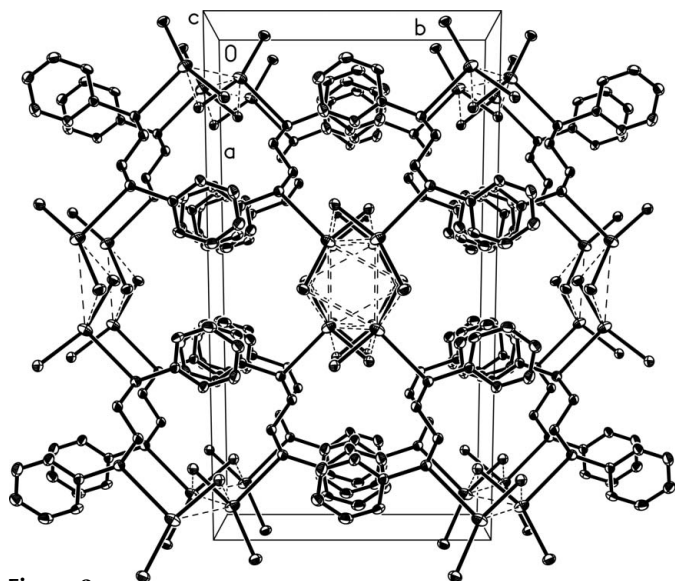
Recently, the crystal structures of two  $\text{Hg}^{\text{II}}$  complexes with flexible dithioether ligands, 1,4-bis(ethylsulfanyl)butane (Liu *et al.*, 2005) and 1,4-bis(benzylsulfanyl)butane (Che *et al.*, 2005), have been reported. These two complexes contain different structural features, *viz.* pseudo-two-dimensional layers and one-dimensional chains, and the two  $\text{Br}^-$  anions around each  $\text{Hg}^{\text{II}}$  center in the two complexes have different coordination modes, *viz.* both  $\mu_2$ -bridging, with one mono-terminal and one  $\mu_2$ -bridging. Even so, there have been fewer structural investigations of  $\text{Hg}^{\text{II}}$ -dithioether complexes than those of  $\text{Ag}^{\text{I}}$  complexes (Bu *et al.*, 2002; Li *et al.*, 2005). We report here a dinuclear  $\text{Hg}^{\text{II}}$  complex,  $[(\text{HgBr}_2)_2L]$ , (I), with a 1,2-bis(phenylsulfanyl)ethane (*L*) ligand.



As shown in Fig. 1, the title complex, (I), has a centrosymmetric dinuclear structure which is formed by one *L* ligand linking two  $\text{HgBr}_2$  units with an inversion center located at the mid-point of the central C—C bond. Each  $\text{Hg}^{\text{II}}$  ion is coordinated by two  $\text{Br}^-$  anions and one S atom of ligand *L*, showing a near T-shape geometry, as exhibited by the relevant bond angles listed in Table 1. The  $\text{Hg}^{\text{II}}$  ion deviates from the coordination plane (Br1/Br2/S1) by 0.0314 (7) Å. In the ligand *L*, the C and S atoms between the two terminal phenyl groups are coplanar, and form a dihedral angle of 100.8 (7)° with the phenyl plane, and 150.5 (8)° with the coordination plane mentioned above. In (I), the *L*-bridged  $\text{Hg} \cdots \text{Hg}$  distance is 8.777 (8) Å, and the  $\text{S} \cdots \text{S}$  distance within one *L* is 4.431 (7) Å.



**Figure 1**  
The structure of (I), showing displacement ellipsoids drawn at the 40% probability level [symmetry code: (A)  $-\frac{1}{2} - x, \frac{1}{2} - y, -1 + z$ ].



**Figure 2**  
Three-dimensional framework structure of (I). Dashed lines indicate weak interactions. H atoms have been omitted.

It should be noted that in the crystal structure of (I), such dinuclear molecules are further linked by  $\text{Br} \cdots \text{Hg}$  weak interactions to form a three-dimensional framework (Fig. 2), with  $\text{Br} \cdots \text{Hg}$  distances in the range 3.263 (7)–3.576 (8) Å. Simultaneously, there also exist weak  $\pi$ – $\pi$  interactions between phenyl groups of adjacent dinuclear molecules with a  $\text{Cg}^i \cdots \text{Cg}^j$  distance of 4.041 (6) Å,  $\text{Cg}^i \cdots \text{perp}$  distances of 3.596 (7) and 3.570 (7) Å, and a dihedral angle of 9.39 (7)° [perp = perpendicular; symmetry code: (i)  $x, 1 - y, -\frac{1}{2} + z$ ].

## Experimental

1,2-Bis(phenylsulfanyl)ethane (*L*) was synthesized *via* the literature method of Hartley *et al.* (1979). To a solution of *L* (50 mg, 0.2 mmol) in chloroform (10 ml) was added a solution of  $\text{HgBr}_2$  (72 mg, 0.2 mmol) in acetone (10 ml). The mixture was filtered and left to stand at room temperature. Colorless single crystals suitable for X-ray investigation were collected after two weeks (yield: 60%).

## Crystal data

$[\text{Hg}_2\text{Br}_4(\text{C}_{14}\text{H}_{14}\text{S}_2)]$   
 $M_r = 967.20$   
 Monoclinic,  $C2/c$   
 $a = 22.0328$  (13) Å  
 $b = 11.6648$  (7) Å  
 $c = 8.0759$  (4) Å  
 $\beta = 103.313$  (4)°  
 $V = 2019.8$  (2) Å<sup>3</sup>  
 $Z = 4$

$D_x = 3.181$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 3720 reflections  
 $\theta = 2.8$ – $27.3$ °  
 $\mu = 23.30$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colorless  
 $0.18 \times 0.16 \times 0.16$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1998)  
 $T_{\min} = 0.284$ ,  $T_{\max} = 1.000$   
 8500 measured reflections

1987 independent reflections  
 1772 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$   
 $\theta_{\max} = 26.0$ °  
 $h = -27 \rightarrow 27$   
 $k = -14 \rightarrow 11$   
 $l = -9 \rightarrow 9$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.098$   
 $S = 1.07$   
 1987 reflections  
 101 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 9.9952P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 2.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.62$  e Å<sup>-3</sup>  
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.00211 (15)

**Table 1**

Selected geometric parameters (Å, °).

Hg1–Br2	2.4404 (8)	Hg1–S1	2.8963 (17)
Hg1–Br1	2.4592 (7)		
Br2–Hg1–Br1	158.41 (3)	C1–S1–C7	101.7 (3)
Br1–Hg1–S1	94.05 (4)	C1–S1–Hg1	114.4 (2)
Br2–Hg1–S1	107.47 (4)	C7–S1–Hg1	99.4 (2)

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with  $\text{C}–\text{H} = 0.93$  or  $0.97$  Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The highest density peak and deepest hole in the final difference map were located 0.89 and 0.77 Å, respectively, from atom Hg1.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT and SHELXTL (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL.

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