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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.013 \text{ \AA}$   
 R factor = 0.043  
 wR factor = 0.122  
 Data-to-parameter ratio = 23.4

For details of how these key indicators were  
 automatically derived from the article, see  
<http://journals.iucr.org/e>.

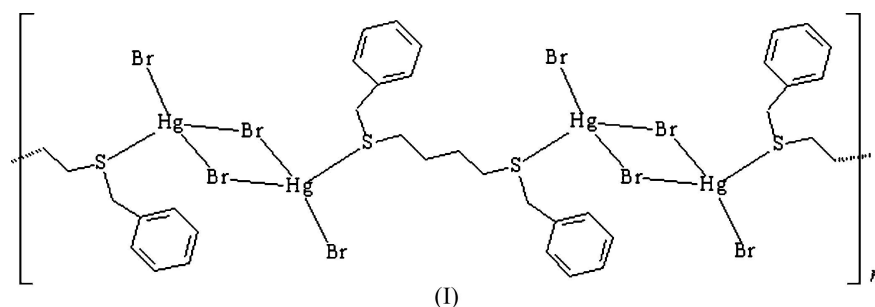
**catena-Poly[[bromomercury(II)]-di- $\mu$ -bromo- $\kappa^4\text{Br}:\text{Br}$ -[bromomercury(II)]- $\mu$ -1,4-bis(benzylsulfanyl)butane- $\kappa^2\text{S}:\text{S}'$ ]**

The title complex,  $[\text{Hg}_2\text{Br}_4(\text{C}_{18}\text{H}_{22}\text{S}_2)]_n$ , has a chain structure. Two bridging Br atoms and two terminal Br atoms coordinate to two  $\text{Hg}^{\text{II}}$  atoms to form a  $(\text{HgBr}_2)_2$  dimer, and the 1,4-bis(benzylsulfanyl)butane ligands bridge the  $(\text{HgBr}_2)_2$  dimers to form a one-dimensional chain. The dimer and butane ligand are each located on inversion centers.  $\text{Hg}^{\text{II}}$  adopts a tetrahedral geometry formed by three Br and one S atoms.

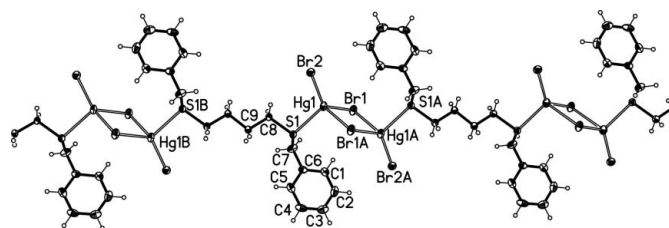
Received 27 October 2005  
 Accepted 22 November 2005  
 Online 26 November 2005

**Comment**

Although thioether ligands can coordinate to the  $\text{Hg}^{\text{II}}$  ion under general reaction conditions,  $\text{Hg}^{\text{II}}$  complexes with thioether have not yet been sufficiently exploited (Liu *et al.*, 2005; Singh *et al.*, 2005; Helm *et al.*, 2003; Noh, 1997) compared to  $\text{Ag}^{\text{I}}$  complexes (Li *et al.*, 2005; Black *et al.*, 1995). Here we report a one-dimensional chain dithioether- $\text{Hg}(\text{II})$  complex,  $[(\text{HgBr}_2)_2L]_n$ , (I) [L is 1,4-bis(benzylsulfanyl)butane].



The title complex, (I), has a one-dimensional chain structure (Fig. 1) formed by L ligands linking  $(\text{HgBr}_2)_2$  dimers. Ligand L is in the normal bridging coordination mode, and dimeric  $(\text{HgBr}_2)_2$  is formed by two Br anions bridging two  $\text{Hg}^{\text{II}}$  cations and two terminal Br anions. The distances between  $\text{Hg}^{\text{II}}$  atoms are 3.884 (2) (within the dimer) and 10.621 (2)  $\text{Å}$



**Figure 1**  
 Part of the polymeric structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry codes: (A) 1 - x, 2 - y, 1 - z; (B) 2 - x, 2 - y, 2 - z].

(across one  $L$ ), respectively. The dimer and  $L$  are each located on inversion centers. The  $\text{Hg}^{\text{II}}$  ion is coordinated by three Br atoms and one S atom from the  $L$  ligand in a tetrahedral geometry with very different bond angles around Hg1 (Table 1).

## Experimental

1,4-Bis(benzylsulfanyl)butane ( $L$ ) was synthesized according to the literature method of Hartley *et al.* (1979). An acetone solution of  $\text{HgBr}_2$  (36 mg, 0.1 mmol) was mixed with a chloroform solution of  $L$  (30 mg, 0.1 mmol). The mixture was stirred for about 30 min at room temperature and then filtered. Colorless single crystals of (I) were obtained after one week.

### Crystal data

$[\text{Hg}_2\text{Br}_4(\text{C}_{18}\text{H}_{22}\text{S}_2)]$   
 $M_r = 511.65$   
 Triclinic,  $P\bar{1}$   
 $a = 7.8468$  (16) Å  
 $b = 8.8428$  (18) Å  
 $c = 9.6395$  (19) Å  
 $\alpha = 70.08$  (3)°  
 $\beta = 75.26$  (3)°  
 $\gamma = 88.53$  (3)°  
 $V = 606.8$  (3) Å<sup>3</sup>

$Z = 2$   
 $D_x = 2.800$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 4964 reflections  
 $\theta = 3.1$ – $27.5$ °  
 $\mu = 19.40$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, colorless  
 $0.20 \times 0.10 \times 0.10$  mm

### Data collection

Rigaku R-AXIS RAPID diffractometer  
 $\omega$  scans  
 Absorption correction: numerical (NUMABS; Higashi, 1995)  
 $T_{\min} = 0.113$ ,  $T_{\max} = 0.247$   
 6034 measured reflections

2759 independent reflections  
 2242 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.047$   
 $\theta_{\max} = 27.5$ °  
 $h = -9 \rightarrow 10$   
 $k = -11 \rightarrow 11$   
 $l = -12 \rightarrow 12$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.122$   
 $S = 1.10$   
 2759 reflections  
 118 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 2.0629P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 1.94$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -2.30$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Hg1–Br1	2.5146 (13)	Hg1–Br2	2.5277 (12)
Hg1–Br1 <sup>i</sup>	2.9649 (14)	Hg1–S1	2.557 (2)
Br1–Hg1–Br1 <sup>i</sup>	90.10 (4)	Br2–Hg1–S1	105.56 (6)
Br1–Hg1–Br2	130.31 (4)	S1–Hg1–Br1 <sup>i</sup>	90.22 (5)
Br1–Hg1–S1	122.56 (6)	Hg1–Br1–Hg1 <sup>i</sup>	89.90 (4)
Br2–Hg1–Br1 <sup>i</sup>	102.14 (4)		

Symmetry code: (i)  $-x + 1, -y + 2, -z + 1$ .

H atoms were placed in calculated positions, with C–H = 0.97 or 0.93 Å, and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The highest peak and deepest hole in the final difference Fourier map are 0.83 and 0.73 Å, respectively, from atom Hg1.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

The authors thank Jilin Normal University for supporting this work.

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