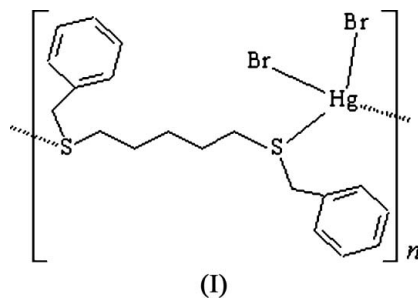


**catena-Poly[[dibromomercury(II)]- $\mu$ -1,5-bis(benzylsulfanyl)pentane- $\kappa^2$ S:S']****Qun Yu, Ying Tao and Jian-Rong Li\***Department of Chemistry, Nankai University,  
Tianjin 300071, People's Republic of ChinaCorrespondence e-mail:  
jianrongli@nankai.edu.cn**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
 $R$  factor = 0.029  
 $wR$  factor = 0.055  
Data-to-parameter ratio = 22.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The title complex,  $[\text{HgBr}_2(\text{C}_{19}\text{H}_{24}\text{S}_2)]_n$ , has a single-chain structure in which adjacent  $\text{HgBr}_2$  units are linked by bridging ligands. The  $\text{Hg}^{\text{II}}$  centre has a distorted tetrahedral coordination environment formed by two  $\text{Br}^-$  anions and two S atoms from distinct ligands.

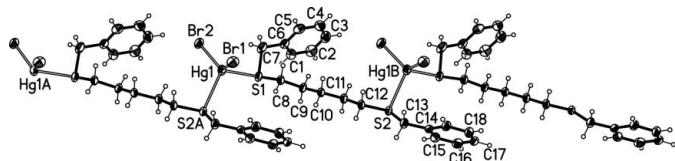
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The structures of  $\text{Ag}^{\text{I}}$  complexes with flexible dithioether ligands have been studied widely by us and others (Blake *et al.*, 1995; Li *et al.*, 2005). However,  $\text{Hg}^{\text{II}}$  complexes with this type of ligand are rare. The crystal structures of two  $\text{Hg}^{\text{II}}$  complexes with 1,4-bis(ethylsulfanyl)butane (Liu *et al.*, 2005) and 1,4-bis(benzylsulfanyl)butane (Che *et al.*, 2005) were reported recently. The former has a pseudo-two-dimensional layer structure, when considering  $\text{Hg}-\text{Br}$  weak coordination, but the latter has a one-dimensional single-chain structure. In these two complexes, the  $\text{Br}^-$  anions have different coordination modes. As a continuation of these studies, we report here the structure of the  $\text{Hg}^{\text{II}}$  title complex, (I), with 1,5-bis(benzylsulfanyl)pentane, *L*, as ligand.



Compound (I) has a one-dimensional chain structure (Fig. 1), in which each *L* ligand links two adjacent  $\text{Hg}^{\text{II}}$  centres, resulting in an intrachain  $\text{Hg} \cdots \text{Hg}$  separation of 10.834 (6) Å. The  $\text{Hg}^{\text{II}}$  atom has a distorted tetrahedral coordination environment (Table 1) formed by two  $\text{Br}^-$  anions and two S atoms from distinct *L* ligands. The  $\text{Br}^-$  anions adopt a mono-terminal coordination mode. There is no obvious weak coordination with other  $\text{Hg}^{\text{II}}$  ions; this is different from the situation in the above-mentioned related complexes.

The bridging skeleton atoms (S1/C8–C12/S2) in *L* are roughly coplanar, with an r.m.s. deviation of 0.046 Å [maximum = 0.0551 (11) Å for S1]. The C13 benzyl group is close to coplanar with the bridging backbone, but the C7 benzyl group is strongly twisted. The dihedral angle between the two benzene ring planes in the same *L* is 36.6 (2)°. It is interesting that in each chain the coordinating S centres have



**Figure 1**  
The structure of (I), showing displacement ellipsoids at the 30% probability level [symmetry codes: (A)  $x - 1, y - 1, z$ ; (B)  $x + 1, y + 1, z$ ].

the same chirality, *S* (or *R*), which leads to each chain being chiral. However, crystal symmetry results in adjacent chains having opposite chirality, and thus the structure as a whole is racemic. The chains in (I) propagate along [110].

## Experimental

1,5-Bis(benzylsulfanyl)pentane (*L*) was synthesized by the method of Hartley *et al.* (1979). An acetone solution (5 ml) of  $\text{HgBr}_2$  (36 mg, 0.1 mmol) was added to 10 ml of a chloroform solution of *L* (32 mg, 0.1 mmol). The mixture was stirred for 20 min and then filtered. The filtrate was left to stand at room temperature for about one week to obtain colourless single crystals of (I) in 57% yield.

### Crystal data

$[\text{HgBr}_2(\text{C}_{19}\text{H}_{24}\text{S}_2)]$	$Z = 2$
$M_r = 676.91$	$D_x = 2.06 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.6155 (15) \text{ \AA}$	Cell parameters from 9068 reflections
$b = 9.4568 (19) \text{ \AA}$	$\theta = 3.1\text{--}27.5^\circ$
$c = 16.227 (3) \text{ \AA}$	$\mu = 10.89 \text{ mm}^{-1}$
$\alpha = 103.52 (3)^\circ$	$T = 293 (2) \text{ K}$
$\beta = 97.15 (3)^\circ$	Block, colourless
$\gamma = 102.04 (3)^\circ$	$0.22 \times 0.18 \times 0.16 \text{ mm}$
$V = 1092.7 (4) \text{ \AA}^3$	

### Data collection

Rigaku R-AXIS RAPID diffractometer	4948 independent reflections
$\omega$ scans	4064 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (NUMABS; Higashi, 1995)	$R_{\text{int}} = 0.026$
$T_{\text{min}} = 0.198, T_{\text{max}} = 0.275$	$\theta_{\text{max}} = 27.5^\circ$
10800 measured reflections	$h = -9 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -21 \rightarrow 17$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.055$   
 $S = 1.06$   
 4948 reflections  
 217 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0161P)^2 + 0.7735P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.77 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.58 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}, ^\circ$ ).

Hg1—Br1	2.5323 (8)	Hg1—S1	2.6303 (15)
Hg1—Br2	2.5165 (8)	Hg1—S2 <sup>i</sup>	2.6346 (11)
C7—S1—C8—C9	−88.2 (3)	C13—S2—C12—C11	−169.2 (3)

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

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 or 0.97  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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## References

- Blake, J. R., Champness, N. R., Levason, W. & Reid, G. (1995). *J. Chem. Soc. Chem. Commun.* pp. 1277–1279.
- Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Che, G.-B., Liu, C.-B., Cui, Y.-C. & Li, C.-B. (2005). *Acta Cryst.* **E61**, m2704–m2705.
- Hartley, F. R., Murray, S. G., Levason, W., Soutter, H. E. & McAuliffe, C. A. (1979). *Inorg. Chim. Acta*, **35**, 265–277.
- Higashi, T. (1995). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
- Li, J.-R., Bu, X.-H., Jiao, J., Du, W.-P., Xu, X.-H. & Zhang, R.-H. (2005). *J. Chem. Soc. Dalton Trans.* pp. 464–474.
- Liu, C.-B., Che, G.-B., Cui, Y.-C. & Li, C.-B. (2005). *Acta Cryst.* **E61**, m2469–m2470.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MS (2002). *CrystalStructure*. Rigaku/MS Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.