

Chun-Bo Liu, Guang-Bo Che,*
Yun-Cheng Cui and Chuan-Bi LiDepartment of Chemistry, Jilin Normal
University, Siping 136000, People's Republic of
ChinaCorrespondence e-mail:
guangbochejl@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.034
 wR factor = 0.082
Data-to-parameter ratio = 24.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[[μ -1,4-bis(ethylsulfanyl)butane- $\kappa^2\text{S},\text{S}'$]-
di- μ -bromo-mercury(II)]

The title complex, $[\text{HgBr}_2L]$ [L is 1,4-bis(ethylsulfanyl)butane, $\text{C}_4\text{H}_9\text{S}$], has a dinuclear structure in which one L ligand links two HgBr_2 units. A C_2 symmetry axis passes through the centre of the ligand L . The Hg^{II} centre adopts a slightly distorted trigonal planar geometry coordinated by two Br^- anions and one S atom from L . When two weak $\text{Hg}-\text{Br}$ interactions are considered, the dinuclear structure expands into a two-dimensional layer containing $[\text{HgBr}_2]_n$ chains, with the Hg^{II} ion having a trigonal-bipyramidal geometry and the Br^- anion acting as a μ_2 linkage.

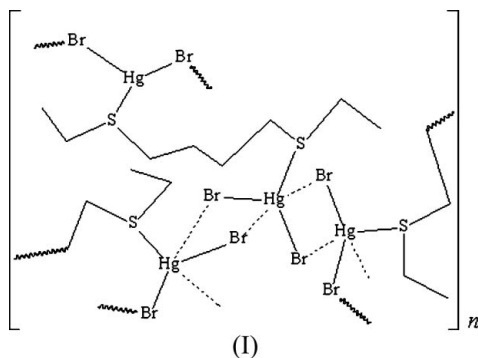
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Comment

Ag^{I} complexes of multi-thioether ligands have been the subject of wide investigation, focused mainly on their structures (Black *et al.*, 1995; Bu *et al.*, 2002; Li *et al.*, 2004). It is well known that the S donors of the thioether ligand can coordinate to the Hg^{II} ion under general reaction conditions. However, in contrast with the Ag^{I} complexes, Hg^{II} complexes with this type of ligand have not been sufficiently exploited (Helm *et al.*, 2003; Noh, 1997). Here, we report the title Hg^{II} complex, (I), with a dithioether ligand, 1,4-bis(ethylsulfanyl)butane (L).



The title complex has a dinuclear structure formed by one L ligand linking two HgBr_2 units (Fig. 1). There is a C_2 symmetry axis in the dinuclear molecule passing through the centre of the L ligand. The Hg^{II} ion is coordinated by two Br atoms and one S atom from the L ligand, showing a slightly distorted trigonal planar geometry, with the bond angles around Hg^{II} in the range $106.51(2)$ – $132.00(2)^\circ$ (Table 1). The Hg^{II} ion deviates from the $\text{Br}1/\text{Br}2/\text{S}1$ plane by $0.1204(2)$ Å. The L ligand acts as a bridging unit linking two Hg^{II} ions; the S–S and Hg–Hg distances are $6.557(2)$ and $8.726(2)$ Å, respectively.

It is interesting that each Hg^{II} centre is weakly coordinated by two Br^- anions of adjacent molecules, with Hg–Br distances of $3.157(2)$ and $3.212(3)$ Å (Table 1), to form a two-

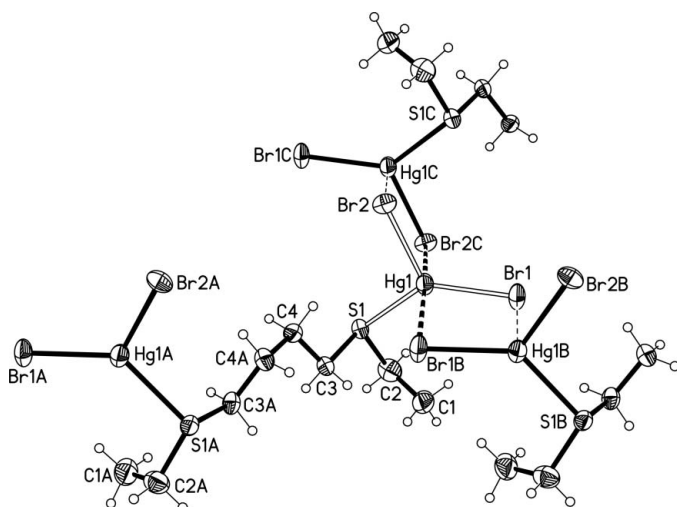


Figure 1
The structure of (I), showing displacement ellipsoids at the 30% probability level. Dashed lines show weak coordinate bonds. [Symmetry codes: (A) $2 - x, y, \frac{1}{2} - z$; (B) $1 - x, y, \frac{1}{2} - z$; (C) $\frac{3}{2} - x, \frac{1}{2} - y, 1 - z$.]

dimensional layer containing $(\text{HgBr}_2)_n$ chains. Thus, the Hg^{II} centre has a trigonal-bipyramidal coordination geometry and each Br^- anion has a μ_2 bridging coordination mode.

Experimental

1,4-Bis(ethylthio)butane (*L*) was synthesized according to the literature method of Hartley *et al.* (1979). The title complex was synthesized by the following procedure. A solution of HgBr_2 (36 mg, 0.1 mmol) in acetone was added to a chloroform solution of *L* (21 mg, 0.1 mmol). The mixture was stirred for about 10 min and then filtered. The filtrate was allowed to evaporate slowly at room temperature. After one week, colourless single crystals of (I) suitable for X-ray investigation were collected (yield 52%).

Crystal data

$[\text{HgBr}_2(\text{C}_4\text{H}_9\text{S})]$	$D_x = 3.245 \text{ Mg m}^{-3}$
$M_r = 449.58$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 6480 reflections
$a = 10.019 (2) \text{ \AA}$	$\theta = 3.2\text{--}27.5^\circ$
$b = 12.952 (3) \text{ \AA}$	$\mu = 25.55 \text{ mm}^{-1}$
$c = 14.798 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 106.56 (3)^\circ$	Cube, colourless
$V = 1840.5 (6) \text{ \AA}^3$	$0.10 \times 0.10 \times 0.10 \text{ mm}$
$Z = 8$	

Data collection

Rigaku R-AXIS RAPID diffractometer	1804 independent reflections
ω scans	1422 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (NUMABS; Higashi, 1995)	$R_{\text{int}} = 0.058$
$T_{\text{min}} = 0.010, T_{\text{max}} = 0.045$	$\theta_{\text{max}} = 26.0^\circ$
7768 measured reflections	$h = -11 \rightarrow 12$
	$k = -15 \rightarrow 15$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.082$
 $S = 1.06$
 1804 reflections
 73 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 4.5708P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.93 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.63 \text{ e \AA}^{-3}$

Table 1
Selected geometric parameters ($\text{\AA}, ^\circ$).

Hg1—S1	2.5050 (8)	Hg1—Br2 ⁱⁱ	3.2123 (8)
Hg1—Br1	2.5190 (6)	S1—C2	1.798 (3)
Hg1—Br1 ⁱ	3.1571 (8)	S1—C3	1.809 (3)
Hg1—Br2	2.5653 (5)		
S1—Hg1—Br1	132.00 (2)	Br2—Hg1—Br1 ⁱ	96.67 (2)
S1—Hg1—Br2	106.51 (2)	Br2—Hg1—Br2 ⁱⁱ	90.84 (2)
Br1—Hg1—Br2	120.80 (1)	Br1 ⁱ —Hg1—Br2 ⁱⁱ	170.20 (1)
S1—Hg1—Br1 ⁱ	96.02 (3)	C2—S1—C3	104.8 (1)
S1—Hg1—Br2 ⁱⁱ	75.74 (3)	C2—S1—Hg1	107.0 (1)
Br1—Hg1—Br1 ⁱ	86.72 (3)	C3—S1—Hg1	107.87 (8)
Br1—Hg1—Br2 ⁱⁱ	94.85 (3)		

Symmetry codes: (i) $-x + 1, y, -z + \frac{1}{2}$; (ii) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 1$.

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with $\text{C—H} = 0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$.

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: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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