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catena-Poly[[bromomercury(II)]-di-μ-bromo-$\kappa^4 Br$:Br-[bromomercury(II)]-μ-1,3-bis(ethylsulfanyl)propane-$\kappa^2 S$:S']

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.033
wR factor = 0.073
Data-to-parameter ratio = 28.2

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

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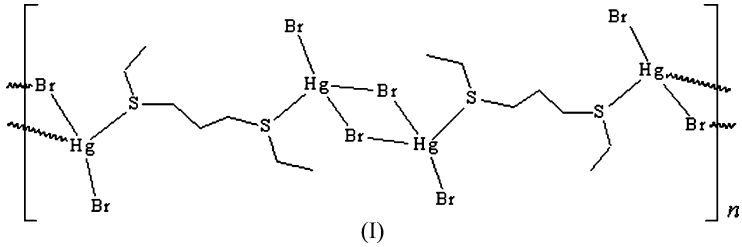
The title complex, $[Hg_2Br_4(C_7H_{16}S_2)]_n$, has a chain structure. Two bridging Br atoms and two terminal Br atoms coordinate to two Hg^{II} atoms, forming an $(HgBr_2)_2$ dimer, which is located on an inversion center. The 1,3-bis(ethylsulfanyl)propane ligands, which lie on a twofold axis, bridge the $(HgBr_2)_2$ dimers, forming a one-dimensional chain. The Hg^{II} atom adopts a tetrahedral geometry, formed by three Br and one S atoms.

Comment

Recently, we and others have reported the crystal structures of some Hg^{II} complexes with flexible dithioether ligands, *viz*. 1,4-bis(ethylsulfanyl)butane (Liu *et al.*, 2005), 1,4-bis(benzylsulfanyl)butane (Che *et al.*, 2005) and 1,2-bis(phenylsulfanyl)ethane (Gong *et al.*, 2006). As a result of differences in the terminal groups and/or spacer lengths of ligands, these complexes display different structural features. In continuation of our work, we report here another one-dimensional chain dithioether–Hg^{II} complex, $[(HgBr_2)_2L]_n$ (L is 1,3-bis(ethylsulfanyl)propane], (I).



(I)

As shown in Fig. 1, the title complex, (I), has a one-dimensional chain structure formed by L ligands linking $(HgBr_2)_2$ dimers. Ligand L is in the normal μ-S,S' bridging coordination mode, and dimeric $(HgBr_2)_2$ is formed by two Br anions bridging two Hg^{II} cations and two terminal Br anions, as observed in the structure of $[Hg_2Br_4$(1,4-bis(benzylsulfanyl)butane)$]_n$ (Che *et al.*, 2005). The distances between Hg^{II} atoms within the dimer and across one L are 3.874 (2) and 6.359 (2) Å, respectively. The dimer is located on an inversion center, but the ligand L lies on a twofold axis. The Hg^{II} ion is coordinated by three Br atoms and one S atom from the L ligand in a distorted tetrahedral geometry, with the bond angles around Hg1 ranging from 91.67 (2) to 127.64 (5)° (Table 1). Compared to (I), the Hg^{II}-1,4-bis(ethylsulfanyl)butane complex (Liu *et al.*, 2005) has a dinuclear structure with different structural parameters. This can be attributed to the difference in the spacer lengths of the two dithioether ligands.

Experimental

1,3-Bis(ethylsulfanyl)propane (*L*) was synthesized according to the literature method of Hartley *et al.* (1979). An acetone solution (10 ml) of $HgBr_2$ (36 mg, 0.1 mmol) was mixed with a chloroform solution (10 ml) of *L* (33 mg, 0.2 mmol). The mixture was stirred and then filtered. The filtrate was allowed to evaporate slowly at room temperature. After one week, colorless single crystals of (I) suitable for X-ray investigation were collected (yield 50%).

Crystal data

$[Hg_2Br_4(C_7H_{16}S_2)]$	$Z = 4$
$M_r = 884.13$	$D_x = 3.445$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 9.818$ (2) Å	$\mu = 27.58$ mm^{-1}
$b = 11.948$ (2) Å	$T = 293$ (2) K
$c = 15.318$ (3) Å	Block, colorless
$\beta = 108.41$ (3)°	0.14 × 0.14 × 0.12 mm
$V = 1704.8$ (6) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	8211 measured reflections
	1943 independent reflections
ω scans	1648 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (*NUMABS*; Higashi,1995)	$R_{int} = 0.062$
	$\theta_{max} = 27.5°$
$T_{min} = 0.121$, $T_{max} = 0.147$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2 + 11.136P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.033$	
$wR(F^2) = 0.073$	
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
1943 reflections	$\Delta\rho_{max} = 1.22$ e Å^{-3}
69 parameters	$\Delta\rho_{min} = -1.65$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Hg1—S1	2.5107 (16)	Hg1—Br2	2.6086 (11)
Hg1—Br1	2.5238 (10)	Hg1—Br2^{i}	2.9409 (8)
S1—Hg1—Br1	127.64 (5)	Br1—Hg1—Br2	116.64 (4)
S1—Hg1—Br2	112.30 (5)	Br1—Hg1—Br2^{i}	95.35 (3)
S1—Hg1—Br2^{i}	100.79 (4)	Br2—Hg1—Br2^{i}	91.67 (2)

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

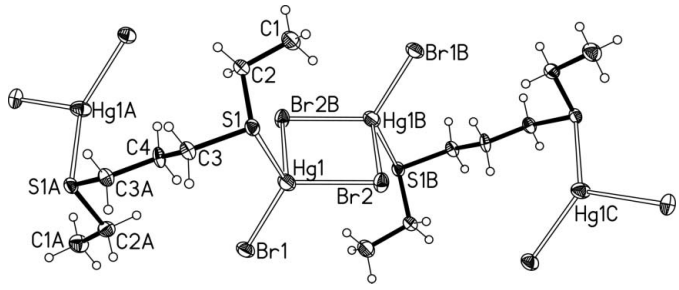


Figure 1
Part of the polymeric structure of (I), showing 30% probability displacement ellipsoids [symmetry codes: (A) $-x, y, \frac{1}{2}-z$; (B) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$; (C) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$].

H atoms were placed in calculated positions (C—H = 0.96 or 0.97 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). The highest peak and deepest hole in the final difference map are 0.73 and 0.71 Å, respectively, from atom Hg1.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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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