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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.016\text{ \AA}$
 R factor = 0.034
 wR factor = 0.067
 Data-to-parameter ratio = 22.4

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

Bis(tetraethylammonium) di- μ -bromobis[dibromomercurate(II)], $(\text{Et}_4\text{N})_2[\text{Hg}_2\text{Br}_6]$

The structure of $(\text{Et}_4\text{N})_2[\text{Hg}_2\text{Br}_6]$ contains dinuclear $[\text{Hg}_2\text{Br}_6]^{2-}$ species as isolated anions. Charge balance is achieved by ordered $[\text{Et}_4\text{N}]^+$ cations. An inversion centre is located at the centre of the $[\text{Hg}_2\text{Br}_6]^{2-}$ unit.

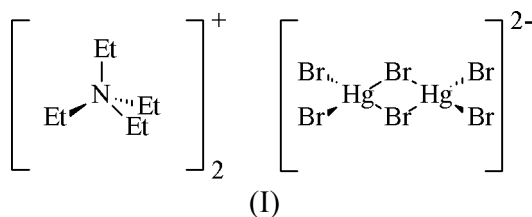
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Comment

The crystal structures of several trihalogenomercurate(II) salts have been reported and show a wide variety of stereochemical arrangements, as listed in a recent overview (Serezhkin *et al.*, 2001). Many different types of halogenomercurate(II) anions were observed, dependent on the stoichiometry as well as on the size and charge of the cation. With the smaller $[\text{Me}_4\text{N}]^+$ cation, for example, the structure consists of trigonal planar $[\text{HgBr}_3]^-$ anions, which are connected into infinite chains by long $\text{Hg}\cdots\text{Cl}$ contacts (White, 1963). The same anionic structure was found for $(\text{Et}_4\text{N})[\text{HgCl}_3]$ (Sandström & Liem, 1978).



The structure of $(\text{Et}_4\text{N})_2[\text{Hg}_2\text{Br}_6]$, (I), contains isolated bitetrahedral $[\text{Hg}_2\text{Br}_6]^{2-}$ units consisting of two tetrahedra

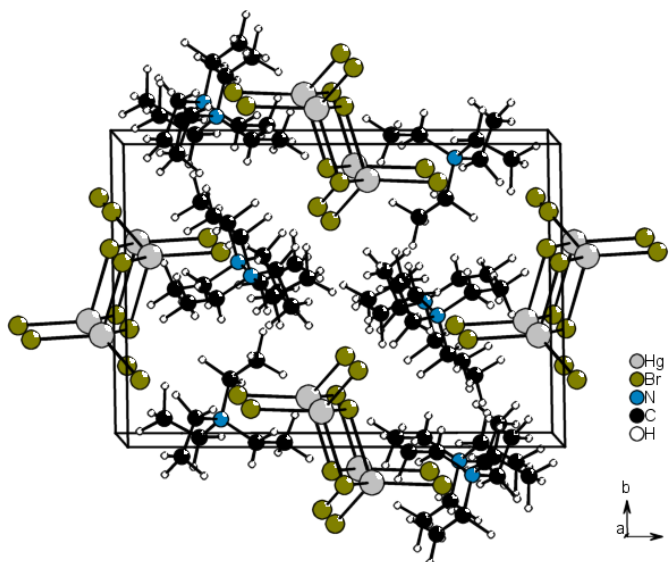


Figure 1
Packing diagram of $(\text{Et}_4\text{N})_2[\text{Hg}_2\text{Br}_6]$, viewed down the a axis.

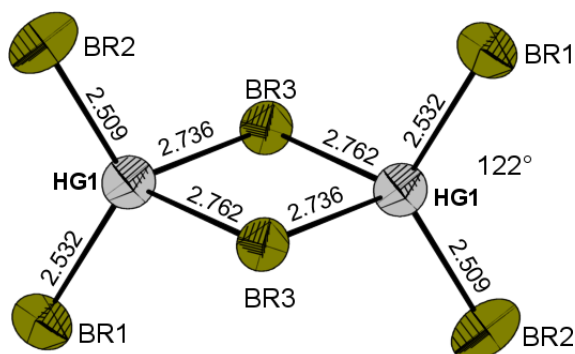


Figure 2
Bitetrahedral $[\text{Hg}_2\text{Br}_6]^{2-}$ units sharing one common edge. Displacement ellipsoids are drawn at the 50% probability level.

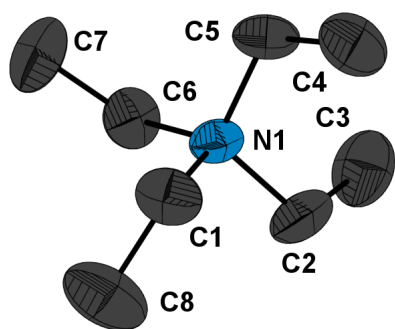


Figure 3
 $[\text{Et}_4\text{N}]^+$ cation. Displacement ellipsoids are drawn at the 50% probability level.

sharing one common edge. Two short bonds of 2.5085 (12) and 2.5319 (13) Å, and two long bonds to the bridging bromide ions of 2.7360 (11) and 2.7618 (11) Å are observed. This type of distorted tetrahedral coordination is also found in other complexes with discrete dimeric $[\text{Hg}_2\text{X}_6]^{2-}$ units ($X = \text{Cl}, \text{Br}, \text{I}$), e.g. in $\text{MgHg}_3\text{Cl}_8 \cdot 6\text{H}_2\text{O}$ (Brodersen *et al.*, 1983), $(\text{Ph}_3\text{AsOH})_2\text{HgBr}_4$ (Harris *et al.*, 1967) and $(\text{NET}_4)[\text{HgI}_3]$ (Goggin *et al.*, 1982). In (I), charge balance is achieved by ordered $[\text{Et}_4\text{N}]^+$ cations (Fig. 3), which are quite remote from the anions, although there are H atoms in the range 2.7–3.1 Å from Br^- , with $\text{Br} \cdots \text{H} - \text{C}$ angles in the range 160–170°. An inversion centre is located at the centre of the $[\text{Hg}_2\text{Br}_6]^{2-}$ unit.

Experimental

1 mmol (0.1717 g) of tetraethylammonium bromide, $(\text{Et}_4\text{N})\text{Br}$, and 1 mmol (0.2715 g) of mercuric bromide, HgBr_2 , were dissolved by stirring in 50 ml methanol at 323 K until a clear solution was obtained. Single crystals were obtained when the solution was allowed to stand at room temperature for 2 d.

Crystal data

$(\text{C}_8\text{H}_{20}\text{N})_2[\text{Hg}_2\text{Br}_6]$
 $M_r = 1141.14$
 Monoclinic, $P2_1/c$
 $a = 9.1148$ (16) Å
 $b = 10.8302$ (13) Å
 $c = 16.140$ (4) Å
 $\beta = 107.377$ (17)°
 $V = 1520.5$ (5) Å³
 $Z = 2$

$D_x = 2.492$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 10 530 reflections
 $\theta = 2.3$ – 25.0°
 $\mu = 17.97$ mm⁻¹
 $T = 293$ (2) K
 Prism, colourless
 0.20 × 0.15 × 0.10 mm

Data collection

Stoe Imaging Plate Diffraction
 System (IPDS-1) diffractometer
 φ scans
 Absorption correction: numerical
 (X -SHAPE; Stoe & Cie, 1998)
 $T_{\min} = 0.051$, $T_{\max} = 0.166$
 10 530 measured reflections

2665 independent reflections
 1450 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.097$
 $\theta_{\max} = 25.0^\circ$
 $h = -10 \rightarrow 10$
 $k = -12 \rightarrow 12$
 $l = -19 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.067$
 $S = 0.81$
 2665 reflections
 119 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0161P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.66$ e Å⁻³
 $\Delta\rho_{\min} = -1.11$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.00203 (12)

Table 1

Selected geometric parameters (Å, °).

Hg1–Br2	2.5082 (12)	N1–C6	1.547 (11)
Hg1–Br1	2.5322 (13)	N1–C2	1.544 (11)
Hg1–Br3 ⁱ	2.7359 (11)	C1–C8	1.509 (13)
Hg1–Br3	2.7618 (11)	C2–C3	1.525 (14)
N1–C5	1.514 (11)	C4–C5	1.521 (14)
N1–C1	1.521 (11)	C6–C7	1.493 (13)
Br2–Hg1–Br1	122.15 (5)	C5–N1–C2	110.9 (7)
Br2–Hg1–Br3	109.82 (4)	C1–N1–C2	107.2 (6)
Br1–Hg1–Br3	109.77 (4)	C6–N1–C2	108.8 (7)
Br3 ⁱ –Hg1–Br3	90.82 (3)	N1–C1–C8	115.7 (8)
Hg1 ⁱ –Br3–Hg1	89.18 (3)	C3–C2–N1	113.8 (8)
C5–N1–C1	109.2 (7)	C4–C5–N1	116.1 (7)
C5–N1–C6	108.9 (7)	C7–C6–N1	114.2 (8)
C1–N1–C6	111.9 (7)		

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

H atoms were fixed at calculated positions using the AFIX23 and AFIX33 commands in *SHELXL97* (Sheldrick, 1997). The highest peak is located 0.92 Å from Br1 and the deepest hole 1.09 Å from Hg1.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-STEP32* (Stoe & Cie, 2000); data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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